

Thermo-Calc Documentation Set

Thermo-Calc Version 2020a



Copyright 2020 Thermo-Calc Software AB. All rights reserved.

Information in this document is subject to change without notice. The software described in this document is furnished under a license agreement or nondisclosure agreement. The software may be used or copied only in accordance with the terms of those agreements.

Thermo-Calc Software AB

Råsundavägen 18, SE-169 67 Solna, Sweden

+46 8 545 959 30

documentation@thermocalc.com

www.thermocalc.com

Contents

Installation Guide 1

Installing Thermo-Calc 2

Key to Using this Guide 3

Installation Terminology 4

About the Thermo-Calc Components
To Be Installed 6

What is installed with a Full
Standalone or Full Network
Client Option? 6

Thermo-Calc 6

Databases 6

Software Development Kits
(SDKs) 7

What does the Custom option
allow me to do during an
installation? 7

System Requirements and Platforms
Tested 7

License and Installation Types 9

License and Installation Types 10

About License Keys and Files 10

Standalone Installations (SUNLL) 11

Multi-User Network Installations
(NWL) 11

Consolidated Network
Installations 11

Distributed Network
Installations 12

License Installations on a Server
Network 13

Preparing for Installation 14

First Steps of Installation 15

Default Directory Installation
Locations 15

Thermo-Calc Default Directory
Locations 15

Subnet Information for Network
Licenses 20

macOS Installation Notes 21

Linux Installation Notes 22

openSUSE Administration
(sudo) Users 22

Opening Thermo-Calc in Linux . 22

Standalone Installations 23

Full Standalone Installations 24

Request your license file from
Thermo-Calc Software 24

Download your Thermo-Calc
installation software 24

Run the applicable installation
file for your operating system .. 24

Select the installation type and
upload the license file 26

Install the software and start
using Thermo-Calc 27

Custom Standalone Installations 27

Select the installation mode
and what components to
include or exclude 28

| | | | |
|--------------------------------------------------------------------------|-----------|------------------------------------------------------------------------------|-----------|
| Set the installation directory and choose the license file | 28 | Installing the License Server on Linux | 37 |
| Install the software and start using Thermo-Calc | 30 | Stop any older versions of the License Server | 37 |
| Add New Components to an Existing Installation | 30 | Write a script to start the License Server | 38 |
| Network Client Installations | 32 | Confirm the HOSTNAME variable and open the UDP port | 38 |
| Full Network Client Installations | 33 | Start the License Server | 39 |
| Install the licensing software . | 33 | Thin Client Installations | 39 |
| Complete Steps 1 to 3 of a full standalone installation | 33 | Custom Network Client Installations | 41 |
| Choose the installation type and enter the computer server details | 33 | Install the licensing software . | 41 |
| Set Up the License Manager on Windows | 34 | Complete Steps 1 to 4 of a full standalone installation | 41 |
| Installation Requirements | 34 | Select the installation mode and what components to include or exclude | 41 |
| Installing the License Manager on Windows | 35 | Set the installation directory and the file path to the license | 42 |
| Install the Sentinel RMS License Manager software . | 35 | Install the software and start using Thermo-Calc | 43 |
| Choose the installation directory | 35 | Unattended Network Client Installations | 44 |
| Choose the setup type and install the software | 35 | Create an option file in a text editor to enter the options | 44 |
| Copy the license files to the destination directory | 36 | Go to the directory where the installation file is stored | 44 |
| Reboot or restart the license manager | 36 | Request License Files | 46 |
| Set Up the License Server on Linux . | 36 | Request a License File from Thermo-Calc Software | 47 |
| Installation Requirements | 36 | | |

| | |
|----------------------------------------------------------------------|-----------|
| Getting License Information Using Thermo-Calc | 47 |
| Requesting the License File for Windows or Linux | 48 |
| Requesting the License File for macOS | 50 |
| Troubleshooting | 52 |
| License Errors | 53 |
| Determining the Current License File Directory Path | 54 |
| From Thermo-Calc | 54 |
| Specifying a New Server Name or IP Number | 57 |
| MATLAB® Installation Directory | 58 |
| Firewalls | 59 |
| Client/Server Mismatch | 59 |
| Compare computer names on the client computer and server | 60 |
| Try these options to correct the issue | 60 |
| macOS Installations: Running the License Initialization Script | 61 |
| Linux Installations: Running the License Initialization Script | 62 |
| Uninstalling Thermo-Calc | 64 |
| Uninstalling Thermo-Calc | 65 |
| Uninstalling Standalone Versions of TC-PRISMA | 66 |
| The Thermo-Calc Software | 1 |
| About the Thermo-Calc Software ... | 2 |

| | |
|---------------------------------------------------------|-----------|
| The Thermo-Calc Software | 3 |
| About the Thermo-Calc Add-on Modules | 3 |
| Diffusion Module (DICTRA) | 3 |
| Precipitation Module (TC-PRISMA) | 4 |
| Process Metallurgy Module | 5 |
| Graphical Mode vs Console Mode .. | 5 |
| Graphical Mode Activities vs Console Mode Modules | 7 |
| Graphical Mode vs Console Mode: Calculation Types | 9 |
| About the File Types and Formats .. | 12 |
| Displaying Thermo-Calc License Information | 13 |
| About the Documentation and Examples | 16 |
| Examples, Manuals and Materials Folders | 17 |
| About the PDF Documentation Folder | 20 |
| About the Examples | 23 |
| Examples by Product | 23 |
| Watch the Video Tutorials | 25 |
| Help Resources | 25 |
| 'Online' Help: No Internet Required | 25 |
| Context Help (Graphical Mode Only) | 25 |
| Console Mode Help | 26 |

| | |
|--------------------------------------------------------------------------|-----------|
| Typographical Conventions | 27 |
| Database Files | 30 |
| About the Database Files | 31 |
| Encrypted vs Unencrypted Database Files | 31 |
| Database Initialization File | 31 |
| User Database Files | 31 |
| Custom Databases: GES5 and GES6 Calculation Engine Version | 32 |
| Database Installation Folder | 32 |
| About Cached Database Files | 33 |
| Editing the Database Initialization File or Unencrypted Database File .. | 34 |
| Best Practice Recommendations | 34 |
| Database Checker | 35 |
| Changing Global Settings | 36 |
| General | 37 |
| Graphical Mode - Default Units | 39 |
| Graphical Mode: Activities | 40 |
| Global Settings: System Definer | 41 |
| Database name | 41 |
| Creating a Database Package .. | 42 |
| Clearing a Database Package Message | 43 |
| Global Settings: Equilibrium Calculator | 44 |
| Global Settings: Diffusion | 45 |

| | |
|------------------------------------------------------------|----------|
| Calculator | |
| Global Settings: Precipitation Calculator | 45 |
| Global Settings: Process Metallurgy | 45 |
| Global Settings: Scheil Calculator | 46 |
| Global Settings: Tables | 47 |
| Global Settings: Graphical and Console Mode Plotting | 47 |
| Titles, Legends and Labels | 49 |
| Fonts and Background Colors ... | 51 |
| Lines and Grids | 51 |
| Data Points and Anchors | 53 |
| Plot Area Size | 53 |
| Image Quality | 54 |
| Global Settings: Console Mode Default Appearance | 54 |
| Thermo-Calc User Guide: Graphical Mode | 1 |
| Working in Graphical Mode | 2 |
| The Graphical Mode Desktop Layout | 3 |
| Menu, Toolbar and Keyboard Shortcuts | 4 |
| Organizing the Windows on the Desktop | 6 |
| Projects and Activities | 8 |
| About the Activity Nodes | 9 |
| Activity Successor and Predecessor Nodes | 9 |

| | |
|------------------------------------------------------|-----------|
| Graphical Mode Activity Node Workflow | 12 |
| Creating Activities and Successors .. | 13 |
| Cloning Activities and Trees | 14 |
| Moving Nodes in the Tree and Using the Grid | 15 |
| Node or Window Status Markers .. | 17 |
| My Project and Activity Menus | 18 |
| My Project Node | 18 |
| Activity Node | 19 |
| Saving and Opening Project Files .. | 21 |
| Saving a Project File | 21 |
| Appending a Project | 21 |
| Opening a Project File | 22 |
| The Calculation Types in Graphical Mode | 23 |
| The Quick Start Wizard and Templates | 26 |
| Creating a Project with the Quick Start Wizard | 28 |
| Creating a Project from a Template | 30 |
| Process Metallurgy Template .. | 32 |
| Steel Library TTT Diagram Template | 33 |
| Defining and Using the Activity Nodes | 35 |
| System Definer | 36 |
| Define the System Definer Node | 36 |

| | |
|------------------------------------------|----|
| Configuration Window Settings | 37 |
| About the Material Files | 44 |
| Austenitic Stainless Steel | 45 |
| Duplex Stainless Steel | 46 |
| High Speed Steel | 46 |
| High Temperature Steel | 46 |
| HSLA Steel | 46 |
| Low Carbon Steel | 46 |
| Maraging Steel | 46 |
| Martensitic Stainless Steel | 46 |
| Tool Steel | 46 |
| Training Steel | 47 |
| Equilibrium Calculator | 48 |
| Define the Equilibrium Calculator | 48 |
| Conditions Tab Settings | 49 |
| Calculating and Plotting Functions | 51 |
| Options Tab Settings | 53 |
| Single Equilibrium and Grid .. | 54 |
| One Axis | 56 |
| Phase Diagram | 56 |
| Calculating with a Fixed Phase .. | 57 |
| Binary Calculator | 60 |
| Configuration Window Settings | 60 |
| Calculation Type | 62 |
| Ternary Calculator | 63 |

| | |
|---------------------------------------------------|----|
| Configuration Window Settings | 63 |
| Calculation Type | 64 |
| Scheil Calculator | 66 |
| Classic Scheil Simulation | 66 |
| Scheil Simulation with a Fast Diffuser Element | 66 |
| Scheil Simulation with Back Diffusion | 67 |
| Summary | 68 |
| Define the Scheil Calculator | 69 |
| Configuration Window Settings | 69 |
| Advanced Settings | 72 |
| Property Model Calculator | 75 |
| Property Model Calculator Workflow | 75 |
| About the Property Models in Thermo-Calc | 76 |
| General Models | 76 |
| Calculation Types | 77 |
| Property Model Development Framework | 77 |
| Examples and Video Tutorials | 77 |
| Coarsening Model | 78 |
| Configuration Settings | 78 |
| Particle Coarsening | 79 |
| Driving Force Model | 80 |
| Configuration Settings | 80 |
| Equilibrium Model | 80 |

| | |
|---------------------------------------------------|-----|
| Configuration Settings | 80 |
| Interfacial Energy Model | 81 |
| Configuration Settings | 81 |
| Estimation of Coherent Interfacial Energy | 82 |
| Liquid and Solidus Temperature Model | 82 |
| Configuration Settings | 82 |
| Phase Transition Model | 83 |
| Configuration Settings | 83 |
| Yield Strength Model | 84 |
| Configuration Settings | 84 |
| General Model Settings | 85 |
| Yield Strength Model Settings | 85 |
| Calculation Type Settings | 87 |
| Grid Definition Settings | 88 |
| About the Yield Strength Model | 89 |
| About the Steel Property Models in Thermo-Calc | 99 |
| Martensite Fractions Model | 99 |
| Martensite Temperatures Model | 100 |
| Pearlite Model | 102 |
| Define the Property Model Calculator | 105 |
| Configuration Window Settings | 106 |

| | |
|-------------------------------|-----|
| Diffusion Calculator | 109 |
| Available Graphical Mode | |
| Features | 109 |
| Using the Template | 110 |
| Diffusion Simulation | |
| Template | 111 |
| Diffusion Calculator | 111 |
| Define the Diffusion | |
| Calculator | 112 |
| Conditions Tab Settings | 112 |
| General | 114 |
| Region Settings | 114 |
| Boundary Conditions | 118 |
| Thermal Profile | 120 |
| Options Tab Settings | 121 |
| Simulation Conditions | 121 |
| Default solver | 121 |
| Timestep Control | 123 |
| Classic and Homogenization | |
| Model Settings | 124 |
| Classic Model Specific | 124 |
| Homogenization Model | |
| Specific | 124 |
| About the Homogenization | |
| Functions | 125 |
| Pause, Resume and Cancel | |
| Diffusion Calculations | 126 |
| To Pause and Resume a | |
| Job | 126 |

| | |
|----------------------------------------|-----|
| To Cancel a Job | 127 |
| Precipitation Calculator | 129 |
| Precipitation Module: | |
| Available Graphical Mode | |
| Features | 129 |
| Using the Template | 129 |
| Precipitation Simulation | |
| Template | 131 |
| Precipitation Calculator | 131 |
| Define the Precipitation | |
| Calculator | 132 |
| Conditions Tab Settings | 132 |
| Composition Unit | 134 |
| Matrix Phase | 134 |
| Precipitate Phase | 137 |
| Calculation Type | 142 |
| Particle Size Distribution (PSD) | 144 |
| Accessing the 'Pre-existing | |
| size distribution' settings | 144 |
| Defining the Preexisting | |
| size distribution | 145 |
| Option Tab Settings | 146 |
| Numerical Parameters | 146 |
| Pause, Resume and Cancel | |
| Precipitation Calculations | 148 |
| To Pause and Resume a | |
| Job | 148 |
| To Cancel a Job | 149 |
| About the Process Metallurgy | |
| Module | 150 |

| | | | |
|---------------------------------------------------------------------------------------------|-----|-------------------------------------------------------------------------|-----|
| The Process Metallurgy Calculator | 151 | Defining the Process Metallurgy Calculator | 164 |
| Working with the Process Metallurgy Module | 151 | Add the calculator, select a database and enter a temperature | 164 |
| Working with Material Groups (Steel, Slag and Gas) | 152 | Define the conditions for the steel, slag and gas material groups | 165 |
| Understanding the Grid Definitions Quantities and How These Relate to the Composition | 154 | Select the Calculation Type and associated definitions | 167 |
| Defining the Material Composition | 155 | Add and define a plot or table and run the simulation | 168 |
| Phase Groups | 158 | Conditions Tab | 168 |
| Slag Property Quantities | 158 | Options Tab | 174 |
| Adiabatic Calculations | 159 | Process Material Equilibrium and Grid | 175 |
| Gas Volume Units | 159 | Working with the Material Manager | 176 |
| Calculation of Component Compositions | 159 | Saving a Material | 177 |
| Definition of Partial Pressure of Oxygen | 159 | Deleting a Material | 178 |
| Activities of Slag Components | 160 | Creating a Material Group | 178 |
| Process Metallurgy Slag Properties | 160 | Deleting a Material Group | 178 |
| Equations and References | 161 | Plot Renderer | 179 |
| Adiabatic Calculations: Calculation of the Material Enthalpy | 162 | Configuration Settings | 180 |
| Process Metallurgy Calculator | 163 | Examples of Calculation Type Differences | 181 |
| Conditions and Options Tabs | 163 | Settings | 181 |
| Plots and Tables | 164 | Plot Settings: TTT Mode | 185 |
| | | Diffusion Calculator Plot | 185 |

| | | | |
|----------------------------------------------------------|------------|-------------------------------------------------------------------------|------------|
| Renderer | | Adding Axes to a Diagram | 216 |
| Simplified Mode | 185 | Heat Map, Contour and 3D Plots | 217 |
| Advanced Mode | 188 | Grid Calculations | 217 |
| Plot Renderer | 189 | Uncertainty Calculations | 224 |
| Plot Settings | 189 | About the Uncertainty Calculations | 226 |
| Non-Isothermal Simulations | 191 | Rotating 3D Plots | 231 |
| Table Renderer | 194 | Plot and Table Formatting | 232 |
| Configuration Settings | 197 | Setting Background Colours ... | 233 |
| Experimental File Reader | 200 | Changing the Plot Properties .. | 233 |
| Scheduler and Event Log | | Plot Labels | 234 |
| Windows | 201 | Plot Labels: Entering a Mixture of Plain Text and Equations | 234 |
| Using the Scheduler | 202 | Plot Labels: Rotation Angle and Show Anchor | 235 |
| Event Log Window | 203 | Moving Plot Labels | 236 |
| Working with Plots and Tables | 204 | About Legend Styles | 236 |
| Performing Projects, Trees and Activities | 205 | Legend and Label Styles | 237 |
| Saving and Printing the Output (Graphical Mode) | 205 | Legend Styles | 237 |
| Saving Diagrams | 206 | Label Styles | 237 |
| Saving Tables | 207 | Graphical Mode Examples | 239 |
| Printing Output | 207 | Thermo-Calc Graphical Mode Examples Collection | 240 |
| Zooming In and Out | 207 | T_01: Calculating a Single- Point Equilibrium | 240 |
| Resetting a Plot to the Default View | 208 | T_02: Stepping in Temperature in the Fe-C System | 242 |
| Plotting Options | 209 | | |
| Plotting Several Calculations in One Diagram | 212 | | |
| Merging Plots into One Diagram | 214 | | |

| | |
|-----------------------------------------------------------------------|-----|
| T_03: Fe-C Phase Diagrams ... | 244 |
| T_04: Fe-Cr-C Ternary Phase Diagram at 1000 K | 246 |
| T_05: Stable and the Metastable Fe-C Phase Diagrams | 249 |
| T_06: Serially Coupled Equilibrium Calculators | 251 |
| Table Renderer Results | 251 |
| T_07: User-Defined Functions .. | 256 |
| T_08: Scheil and Equilibrium Solidification | 258 |
| T_09: Carbide Driving Force Heat Map | 262 |
| T_10: Scheil Solidification with Back Diffusion | 263 |
| Thermo-Calc Property Model Examples Collection | 265 |
| PM_G_01: Phase Transition ... | 265 |
| PM_G_02: Coarsening and Interfacial Energy | 267 |
| Plot Results | 267 |
| PM_G_03: Driving Force and Interfacial Energy | 271 |
| PM_G_04_Yield_Strength | 273 |
| PM_G_05_Yield_Strength_ NiAlCr | 276 |
| PM_G_06_Yield_Strength_ HEA | 279 |
| PM_Fe_01: Fe-Cr-C Martensite with Intercritical Annealing | 281 |

| | |
|-------------------------------------------------------------------------------------|-----|
| PM_Fe_02: Fe-Mn Martensite Morphologies | 283 |
| PM_Fe_03: Fe-C-Mn Pearlite .. | 284 |
| Process Metallurgy Examples Collection | 288 |
| PMET_01: Basic Oxygen Furnace (BOF) | 288 |
| Amount of Phase Groups | 289 |
| Composition of Liquid Metal | 290 |
| Composition of Liquid Slag .. | 292 |
| PMET_02: Ladle Furnace | 294 |
| Fraction of Liquid Slag | 296 |
| Sulfur in Liquid Steel | 297 |
| Ratio of Liquid Slag and Sulfur in Liquid Steel | 298 |
| PMET_03_Argon_Oxygen_ Decarburization | 301 |
| Slag Basicity | 303 |
| S Content in Steel | 304 |
| Cr Content in Slag | 305 |
| Amount of Slag | 306 |
| Liquid Slag Fraction | 307 |
| Diffusion Module (DICTRA) Graphical Mode Examples | 308 |
| D_01 Homogenization of a Binary Fe-Ni Alloy | 308 |
| D_02 Ferrite(bcc)/Austenite (fcc) Transformation in a Binary Fe-C Alloy | 310 |

| | |
|----------------------------------------------------------------------------------------------------|-----|
| D_03 Evolution of an Fe-Cr-Ni Diffusion Couple | 313 |
| D_04 Fe-C Moving Boundary: Austenite to Ferrite | 314 |
| D_05 $\gamma/\alpha/\gamma$ Diffusion couple of Fe-Ni-Cr alloys | 317 |
| D_06 Diffusion Through a Tube Wall | 323 |
| D_07 Multiphase Carburization of a Ni-25Cr- 0.0001C alloy | 326 |
| Precipitation Module (TC- PRISMA) Graphical Mode Examples | 330 |
| P_01: Isothermal Precipitation of Al3Sc | 330 |
| Tutorial-P_01-Isothermal | 333 |
| P_02: Stable and Metastable Carbides - Isothermal | 340 |
| P_03: Stable and Metastable Carbides - TTT Diagram | 342 |
| P_04: Precipitation of Iron Carbon Cementite | 345 |
| P_05: Precipitation of γ' in Ni Superalloys - Isothermal | 347 |
| P_06: Precipitation of γ' in Ni Superalloys - Non-isothermal | 350 |
| P_07: Continuous Cooling Transformation (CCT) Diagram of Ni-Al-Cr γ - γ' | 355 |
| Tutorial-P_07-CCT | 357 |
| P_08: Precipitation of Cu-Ti | 362 |

| | |
|-----------------------------------------------------------------------------------------------------|-----|
| CU4Ti with Assumptions of Sphere and Needle Morphologies | |
| P_09: Precipitation of Al-Sc AL3SC with Assumption of Sphere and Cuboid Morphologies | 367 |
| Tutorial-P_09-Al-Sc-Sphere_ Cuboid | 374 |
| P_10: Initial Particle Size Distribution of Fe-Cr-C | 383 |
| Volume Fraction with Initial Particle Size Distribution | 386 |
| Volume Fraction with No Initial Particle Size Distribution | 386 |
| P_11: Interfacial Energy Function | 387 |
| Mean Radius | 388 |
| P_12: Comparing Growth Rate Models for an Al-Zr System | 389 |
| Mean Radius | 391 |
| P_13: Paraequilibrium Precipitation of Cementite Fe- C-Cr | 391 |
| Mean Radius | 393 |

Thermo-Calc Property Model Development Framework 1

| | |
|-------------------------------------------------------------------|---|
| Introduction to the Property Model Development Framework | 2 |
|-------------------------------------------------------------------|---|

| | |
|------------------------------------------------|---|
| Property Model Installation Directory | 3 |
|------------------------------------------------|---|

| | |
|---------------------------------------------------|-----------|
| Creating a Custom Property Model . | 3 |
| PDF: Property Model Framework Guide | 5 |
| Thermo-Calc User Guide: Console Mode | 1 |
| Working in Console Mode | 1 |
| The Console Mode Layout | 2 |
| Console Window | 3 |
| Console Mode Results Window | 4 |
| Event Log Window | 4 |
| Keyboard Shortcuts to Navigate Between Tabs | 4 |
| Modules and Commands | 6 |
| Console Mode Workflow | 7 |
| Defining a System in Console Mode | 8 |
| Console Mode Modules | 9 |
| Moving Between Modules and Submodules | 13 |
| Entering Command Names or Abbreviations | 14 |
| Using the Command Line Prompt | 15 |
| Main Menu Commands | 15 |
| Command History | 16 |
| Wild Card Characters | 17 |
| File Types | 19 |
| Working with the Console Mode File Types | 20 |
| Opening Console Mode Macro Files | 20 |

| | |
|-------------------------------------------------------------------|-----------|
| Opening a Macro from the Main Menu | 21 |
| Opening a Macro Using a Command | 22 |
| Drag and Drop a Macro File into the Console Window | 22 |
| Log Files | 23 |
| Macro Files | 24 |
| Workspace Files | 26 |
| Links to Workspace Commands in Various Modules | 27 |
| Editing the Default Console Directory | 29 |
| Experimental Data Files (*.POP, *.DOP) | 31 |
| Calculations | 35 |
| About the Gibbs Energy System (GES) Module | 36 |
| Calculation Engine: GES5 vs GES6 | 36 |
| Equilibrium Calculations | 38 |
| The Equilibrium Calculation Module (POLY3) | 39 |
| Setting Conditions for Equilibrium Calculations | 40 |
| Calculating an Equilibrium | 42 |
| Calculating an Equilibrium with a Fixed Phase | 43 |
| Calculating an Equilibrium with Suspended or Dormant Phases | 43 |
| Property Diagrams | 45 |

| | | | |
|---------------------------------------------------------------|----|------------------------------------------------------------------|----|
| About Property Diagrams | 46 | About Potential Diagrams | 67 |
| Calculating and Plotting a Property Diagram | 46 | POTENTIAL_DIAGRAM | 67 |
| Calculating a Property Diagram One Phase at a Time | 48 | Calculating a Potential Diagram | 68 |
| Calculating Several Properties in the Same Diagram | 49 | Calculating a Potential Diagram with Different Pressure | 69 |
| Phase Diagrams | 50 | Scheil Simulations | 71 |
| About Phase Diagrams | 51 | About the Scheil-Gulliver Solidification Simulations | 72 |
| Calculating and Plotting a Phase Diagram | 51 | Classic Scheil Simulation | 72 |
| About Binary Phase Diagrams .. | 53 | Scheil Simulation with a Fast Diffuser Element | 72 |
| BINARY_DIAGRAM | 54 | Scheil Simulation with Back Diffusion | 73 |
| About Ternary Phase Diagrams | 54 | Summary | 74 |
| TERNARY_DIAGRAM | 56 | Simulating a Scheil Solidification Process | 75 |
| About Quasi-Binary and Quasi- Ternary Phase Diagrams | 56 | Scheil Module State Variables .. | 78 |
| Calculating a Quasi-Binary Phase Diagram | 57 | Scheil Module Frequently Asked Questions | 79 |
| Calculating a Quasi-Ternary Phase Diagram | 58 | Aqueous Solutions and Pourbaix Diagrams | 81 |
| T0 Temperature Simulations | 59 | About Aqueous Solutions and the Pourbaix Diagram | 82 |
| About T0 Temperature Simulations | 60 | Calculating a Pourbaix Diagram | 84 |
| Making a T0 Temperature Simulation | 60 | Plotting More Pourbaix Diagrams | 86 |
| Paraequilibrium | 62 | Stepping Calculations in an Aqueous Solution | 88 |
| About Paraequilibrium | 63 | POURBAIX_DIAGRAM Module .. | 89 |
| Calculating a Paraequilibrium .. | 63 | Getting started with the Pourbaix module | 90 |
| Potential Diagrams | 66 | | |

| | | | |
|---------------------------------------------------------------------|-----------|----------------------------------------------------------|------------|
| What is a Pourbaix diagram? | 90 | Working with the Console Mode Output | 108 |
| What database should I use? | 90 | Pause, Resume or Stop Output to the Console Window | 108 |
| Choosing a custom aqueous solution database | 90 | Controlling Console Output | 109 |
| Copy and Rename the POLY3 file | 92 | Commands by Module | 110 |
| Enforce a Pause | 92 | System Utilities (SYS) Commands .. | 111 |
| Pourbaix Main Options | 93 | ABOUT | 112 |
| Tabulation Reactions | 94 | BACK | 112 |
| About the Tabulation Reaction Module | 95 | CLOSE_FILE | 112 |
| Tabulating a Reaction | 96 | DISPLAY_LICENSE_INFO | 112 |
| Tabulating a Substance or Solution Phase at Fixed Composition | 97 | EXIT | 113 |
| Results | 99 | GOTO_MODULE | 113 |
| Console Mode Results | 100 | HELP (? and ??) | 113 |
| Using the POST Module | 101 | HELP | 113 |
| Plotting Diagrams | 101 | HP_CALCULATOR | 114 |
| Saving and Printing the Output in Console Mode | 102 | INFORMATION | 114 |
| Commands to Save and Print Diagrams | 103 | MACRO_FILE_OPEN | 114 |
| Commands to Save Tables | 104 | OPEN_FILE | 117 |
| Saving Diagrams | 104 | SET_COMMAND_UNITS | 117 |
| Printing Diagrams | 105 | SET_ECHO | 118 |
| Modifying Diagrams | 106 | SET_GES_VERSION | 118 |
| Loading Saved Diagrams | 108 | SET_INTERACTIVE | 119 |
| | | SET_INTERACTIVE_MODE | 119 |
| | | SET_LOG_FILE | 119 |
| | | SET_PLOT_ENVIRONMENT | 120 |
| | | SET_TC_OPTIONS | 120 |

| | | | |
|-----------------------------|-----|---------------------------|-----|
| STOP_ON_ERROR | 121 | LIST_PHASE_ADDITION | 140 |
| Database (TDB) Module | | NEW_COMPOSITION_SET ... | 141 |
| Commands | 122 | MAJOR_CONSTITUENTS | 142 |
| AMEND_SELECTION | 123 | NEW_COMPOSITION_SET ... | 143 |
| APPEND_DATABASE | 123 | OUTPUT_FILE_FOR_SHOW .. | 144 |
| DATABASE_INFORMATION | 123 | PARAEQUILIBRIUM | 144 |
| DEFINE_ELEMENTS | 124 | PHASE_ADDITION | 147 |
| DEFINE_SPECIES | 124 | PRESENT_PHASE | 148 |
| DEFINE_SYSTEM | 125 | SHOW_FOR_T= | 148 |
| GET_DATA | 126 | STABILITY_CHECK | 149 |
| LIST_DATABASE | 126 | TOGGLE_ALTERNATE_ | |
| LIST_SYSTEM | 127 | MODE | 150 |
| REJECT | 127 | T-ZERO_TEMPERATURE | 150 |
| RESTORE | 128 | AMEND_STORED_EQUILIBRIA | 151 |
| SET_AUTO_APPEND_ | | CHANGE_STATUS | 152 |
| DATABASE | 129 | COMPUTE_EQUILIBRIUM | 156 |
| SWITCH_DATABASE | 130 | COMPUTE_TRANSITION | 158 |
| POLY Module Commands | 131 | CREATE_NEW_EQUILIBRIUM .. | 159 |
| ADD_INITIAL_EQUILIBRIUM ... | 133 | DEFINE_COMPONENTS | 160 |
| ADVANCED_OPTIONS | 135 | DEFINE_DIAGRAM | 161 |
| STEP_AND_MAP | 136 | DEFINE_MATERIAL | 163 |
| EQUILIBRIUM_CALCUL | 137 | DELETE_INITIAL_ | |
| Settings for the | | EQUILIBRIUM | 166 |
| Minimization of an | | DELETE_SYMBOL | 167 |
| Equilibria | 137 | ENTER_SYMBOL | 167 |
| GLOBAL_MINIMIZATION | 139 | EVALUATE_FUNCTIONS | 170 |
| KEEP_COMP_SET_ | | LIST_AXIS_VARIABLE | 170 |
| NUMBERS | 140 | | |

| | |
|---------------------------------------------|-----|
| LIST_CONDITIONS | 170 |
| LIST_EQUILIBRIUM | 171 |
| LIST_INITIAL_EQUILIBRIA | 172 |
| LIST_STATUS | 172 |
| LIST_SYMBOLS | 173 |
| LOAD_INITIAL_EQUILIBRIUM | 173 |
| MAP | 173 |
| POST | 175 |
| READ_WORKSPACES | 176 |
| REINITIATE_MODULE | 176 |
| SAVE_WORKSPACES | 176 |
| SELECT_EQUILIBRIUM | 178 |
| SET_ALL_START_VALUES | 178 |
| SET_AXIS_VARIABLE | 180 |
| SET_CONDITION | 181 |
| SET_INPUT_AMOUNTS | 183 |
| SET_NUMERICAL_LIMITS | 184 |
| SET_REFERENCE_STATE | 185 |
| SET_START_CONSTITUTION | 187 |
| SET_START_VALUE | 187 |
| SHOW_VALUE | 188 |
| STEP_WITH_OPTIONS | 188 |
| TABULATE | 201 |
| Gibbs Energy System (GES) Commands | 202 |
| ADD_COMMENT | 204 |
| AMEND_ELEMENT_DATA | 204 |

| | |
|----------------------------------------------------|-----|
| AMEND_PARAMETER | 205 |
| Solution Models in the GIBBS (GES) Module | 207 |
| AMEND_PHASE_ DESCRIPTION | 214 |
| AMEND_SYMBOL | 218 |
| CHANGE_STATUS | 220 |
| ENTER_ELEMENT | 221 |
| ENTER_FUNCTION | 222 |
| ENTER_PARAMETER | 223 |
| About the ENTER_PHASE Command | 225 |
| ENTER_PHASE | 228 |
| ENTER_SPECIES | 230 |
| ENTER_SYMBOL | 231 |
| LIST_CONSTITUTION | 235 |
| LIST_DATA | 235 |
| LIST_PARAMETER | 236 |
| LIST_PHASE_DATA | 237 |
| LIST_STATUS | 237 |
| LIST_SYMBOL | 240 |
| READ_GES_WORKSPACE | 241 |
| READ_WORKSPACES | 241 |
| RECOVER_START_VALUES | 242 |
| REINITIATE | 242 |
| SAVE_GES_WORKSPACE | 243 |
| SAVE_WORKSPACES | 243 |
| SET_R_AND_P_NORM | 245 |

| | |
|------------------------------|-----|
| SCHEIL Module Commands | 246 |
| BCC_TO_FCC_ | |
| TRANSFORMATION | 247 |
| EVALUATE_SEGREGATION_ | |
| PROFILE | 247 |
| GLOBAL_MINIMIZATION | 248 |
| LIQUID_PHASE_NAME | 248 |
| SAVE_FILE_NAME | 248 |
| SET_NUMERICAL_LIMITS | 249 |
| START_WIZARD | 250 |
| TEMPERATURE_STEP | 253 |
| TERMINATION_CRITERIA | 253 |
| USE_BACK_DIFFUSION | 253 |
| PARROT Module Commands | 255 |
| AMEND_PARAMETER | 257 |
| AMEND_SYMBOL | 259 |
| COMPILE_EXPERIMENTS | 261 |
| CONTINUE_OPTIMIZATION | 262 |
| CREATE_NEW_STORE_FILE | 263 |
| EDIT_EXPERIMENTS | 263 |
| About the ENTER_PARAMETER | |
| Command | 264 |
| Defining the Parameter | 264 |
| ENTER_PARAMETER | 268 |
| LIST_ALL_VARIABLES | 270 |
| LIST_CONDITIONS | 270 |
| LIST_PARAMETER | 271 |
| LIST_PHASE_DATA | 272 |

| | |
|--------------------------------|-----|
| LIST_RESULT | 272 |
| LIST_STORE_FILE | 276 |
| LIST_SYMBOL_IN_GES | 276 |
| OPTIMIZE_VARIABLES | 277 |
| READ_PARROT_WORKSPACES | 277 |
| RECOVER_VARIABLES | 278 |
| REINITIATE | 278 |
| RESCALE_VARIABLES | 278 |
| SAVE_PARROT_WORKSPACES | 278 |
| SET_ALTERNATE_MODE | 279 |
| SET_EXTERNAL_PARAMETER | 279 |
| SET_FIX_VARIABLE | 280 |
| SET_OPTIMIZING_CONDITION | 281 |
| SET_OPTIMIZING_VARIABLE | 282 |
| SET_OUTPUT_LEVELS | 283 |
| SET_SCALED_VARIABLE | 283 |
| SET_STORE_FILE | 284 |
| EDIT_EXPERIMENTS (ED_EXP) | |
| Submodule Commands | 285 |
| ADVANCED_OPTIONS | 287 |
| CHANGE_STATUS | 287 |
| COMMENT | 291 |
| COMPUTE_ALL_EQUILIBRIA | 291 |
| CREATE_NEW_EQUILIBRIUM | 292 |
| DEFINE_COMPONENTS | 293 |
| DELETE_SYMBOL | 293 |
| ENTER_SYMBOL | 294 |

| | |
|-------------------------------|-----|
| EVALUATE_FUNCTIONS | 296 |
| EXPERIMENT | 296 |
| EXPORT | 298 |
| FLUSH_BUFFER | 298 |
| GRAPHICS_PLOT | 299 |
| IMPORT | 299 |
| LABEL_DATA | 300 |
| LIST_ALL_EQUILIBRIA | 300 |
| LIST_CONDITIONS | 301 |
| LIST_EQUILIBRIUM | 301 |
| LIST_STATUS | 302 |
| LIST_SYMBOLS | 303 |
| MAKE_POP_FILE | 303 |
| READ_WORKSPACES | 304 |
| REINITIATE_MODULE | 304 |
| RESTORE_ALL_WEIGHTS | 305 |
| SAVE_WORKSPACES | 305 |
| SELECT_EQUILIBRIUM | 306 |
| SET_ALL_START_VALUES | 306 |
| SET_ALTERNATE_CONDITION | 307 |
| SET_CONDITION | 310 |
| SET_NUMERICAL_LIMITS | 312 |
| SET_REFERENCE_STATE | 313 |
| SET_START_CONSTITUTION | 315 |
| SET_START_VALUE | 315 |
| SET_WEIGHT | 316 |

| | |
|-------------------------------------------------|-----|
| SHOW_VALUE | 317 |
| STORE_ALL_WEIGHTS | 318 |
| TABLE_HEAD, TABLE_VALUES and TABLE_END | 318 |
| TRANSFER_START_VALUES | 320 |
| Tabulation Reaction (TAB) Commands | 321 |
| ENTER_FUNCTION | 322 |
| ENTER_REACTION | 323 |
| LIST_SUBSTANCES | 324 |
| SET_ENERGY_UNIT | 327 |
| SET_PLOT_FORMAT | 327 |
| SWITCH_DATABASE | 327 |
| TABULATE | 329 |
| TABULATE_DERIVATIVES | 329 |
| TABULATE_REACTION | 333 |
| TABULATE_SUBSTANCE | 336 |
| REACTOR (REACTOR_ SIMULATOR) Commands | 342 |
| CREATE_DIVIDERS | 343 |
| CREATE_PIPES | 343 |
| CREATE_STAGE_BOXES | 344 |
| EXECUTE_POLY3_COMMAND | 345 |
| LIST_RECORDS | 345 |
| READ_WORKSPACE | 346 |
| SAVE_WORKSPACES | 346 |
| START_SIMULATION | 347 |
| POST Module Commands | 350 |

| | |
|-----------------------------|-----|
| ADD_LABEL_TEXT | 352 |
| APPEND_EXPERIMENTAL_ | |
| DATA | 353 |
| CHANGE_LEGEND | 354 |
| DUMP_DIAGRAM | 355 |
| ENTER_SYMBOL | 356 |
| FIND_LINE | 358 |
| LIST_DATA_TABLE | 358 |
| LIST_PLOT_SETTINGS | 359 |
| LIST_SYMBOLS | 359 |
| MAKE_EXPERIMENTAL_ | |
| DATAFILE | 360 |
| MODIFY_LABEL_TEXT | 360 |
| PLOT_DIAGRAM | 361 |
| PRINT_DIAGRAM | 361 |
| QUICK_EXPERIMENTAL_PLOT | 362 |
| REINITIATE_PLOT_SETTINGS .. | 362 |
| RESTORE_PHASE_IN_PLOT | 362 |
| SELECT_PLOT | 362 |
| SET_AXIS_LENGTH | 363 |
| SET_AXIS_PLOT_STATUS | 363 |
| SET_AXIS_TEXT_STATUS | 363 |
| SET_AXIS_TYPE | 364 |
| SET_COLOR | 364 |
| SET_CORNER_TEXT | 365 |
| SET_DIAGRAM_AXIS | 366 |
| SET_DIAGRAM_TYPE | 368 |

| | |
|----------------------------|-----|
| SET_FONT | 368 |
| SET_LABEL_CURVE_OPTION .. | 369 |
| SET_PLOT_FORMAT | 370 |
| SET_PLOT_OPTIONS | 370 |
| SET_PLOT_SIZE | 372 |
| SET_PREFIX_SCALING | 372 |
| SET_RASTER_STATUS | 372 |
| SET_REFERENCE_STATE | 372 |
| SET_SCALING_STATUS | 374 |
| SET_TIC_TYPE | 375 |
| SET_TIELINE_STATUS | 375 |
| SET_TITLE | 375 |
| SET_TRUE_MANUAL_SCALING | 376 |
| SUSPEND_PHASE_IN_PLOT | 376 |
| TABULATE | 376 |

Parameters, Functions and Variables378

Specifying Parameters379

Thermodynamic Variables and Units 381

About Operators and Functions382

Available Operators for Writing Functions382

Thermodynamic Variables383

Common Thermodynamic Variables 383

How to Read the Tables384

| | |
|------------------------------------------------------------------|-----|
| Intensive Variables | 384 |
| Extensive Variables | 385 |
| Special Quantities | 388 |
| The u-Fraction Variable | 389 |
| Suffixes | 390 |
| Normalizing Suffixes | 390 |
| Derived Variables and Partial Derivatives | 395 |
| Defining New Derived Variables and Functions | 397 |
| Derived Variables for Aqueous Solutions | 397 |
| Defining New Derived Variables for Aqueous Solutions | 399 |
| Thermodynamic Variables and Wildcard Characters | 400 |
| Units of State Variables and Derived Variables | 402 |
| User-Specified Units | 402 |
| Examples of User-Defined Units | 402 |
| For intensive variables of a defined system | 403 |
| For extensive variables of a defined system | 403 |
| For intensive variables of a system component | 404 |
| For extensive variables of a system component | 405 |
| For intensive variables of a | 406 |

| | |
|-----------------------------------------------------------------------|------------|
| species in a phase | |
| For extensive variables of a species in a phase | 407 |
| Technical Notes | 411 |
| Technical Note: Pipe or Redirect Output Data from Console Mode . | 412 |
| Windows | 412 |
| Linux | 412 |
| Mac | 412 |
| Console Mode Examples | 413 |
| Thermo-Calc Console Mode Examples | 414 |
| Binary Phase Diagram Examples .. | 415 |
| Property Diagram Examples | 418 |
| Ternary Phase Diagram Examples | 423 |
| Multicomponent Phase Diagram Examples | 427 |
| Examples Calculating Thermodynamic and Related Quantities | 429 |
| Single Equilibrium Calculation Examples | 432 |
| Potential Diagram Example | 434 |
| Examples of Scheil- Gulliver Calculations | 434 |
| Example Calculating Chemical Ordering | 435 |
| Examples Using the Gibbs Energy System (GES) Module | 436 |
| Notes related to the example | 438 |

| | |
|-------------------------------------------------------------------------------------------------|-----|
| Amending the binary excess model | 438 |
| Amending the ternary extrapolation model | 439 |
| Example Calculating the T0 Temperature | 439 |
| Examples Calculating Paraequilibrium | 439 |
| Example Using Functions and Variables | 441 |
| Example Using the PARROT and EDIT_EXPERIMENT Modules | 441 |
| Pourbaix Module Examples | 444 |
| The PAQ2 Database | 445 |
| Additional Examples in this Series | 445 |
| Step 1: Single-Point Calculations for H2O-NaCl system | 446 |
| Step 2: Single-Point Calculations for Fe-X (X = Cr-Ni-Co) system | 446 |
| Step 3: Single-Point Calculations for Fe-Cr-Ni-Co + H2O-NaCl system | 446 |
| Step 4: Pourbaix Diagram Mapping for Fe-Cr-Ni-Co + H2O-NaCl system - define the variables | 446 |
| Pourbaix Module Examples TCEX40A to 40E | 446 |
| POURBAIX_DIAGRAM Commands for Options 1 to 4 | 450 |

| | |
|-----------------------------------------------------------------------------|----------|
| Option 1: Start a completely new Pourbaix diagram calculation | 450 |
| Chemical system (elements) | 451 |
| Initial bulk composition ... | 451 |
| Option 2: Open an existing file and plot other property diagrams | 456 |
| Option 3: Open an existing file and make another Pourbaix calculation | 457 |
| Option 4: Open an Existing file and make another Stepping calculation | 460 |
| Example Using the Tabulate Reaction (TAB) Module | 462 |
| Example Using the Reactor Module | 462 |
| Application Examples | 463 |
| Data Optimization User Guide | 1 |
| Introduction | 2 |
| Introduction to Data Optimization .. | 3 |
| GES5 and GES6 Calculation Engine Version | 3 |
| Data Optimization | 4 |
| The Least-Squares Method | 4 |
| The CALPHAD Approach | 5 |
| Working with Data Optimization in Thermo-Calc | 7 |
| Data Optimization in Thermo-Calc .. | 8 |

| | | | |
|--------------------------------------------------------------|-----------|--------------------------------------------------------------------|-----------|
| Data Optimization Workflow | 8 | Grouping Equilibria with Labels | 26 |
| The PARROT Module | 9 | Dividing the POP-File into Several Blocks | 26 |
| GES5 and GES6 Calculation Engine Version | 9 | The Setup File | 28 |
| The EDIT_EXPERIMENTS Module ... | 10 | Creating the Setup File | 29 |
| Data Optimization in Other Modules | 10 | Defining the System | 29 |
| Optimization File Types | 10 | Creating Additional Composition Sets of a Phase ... | 30 |
| Optimization Workspaces | 11 | Entering the Optimizing Variables ... | 30 |
| Method for Optimization and Simulation | 12 | Entering Optimizing Variables in Parameter Specifications | 30 |
| Creating the POP-File | 13 | Entering Interaction Parameters | 32 |
| Experimental Information | 14 | Initializing Optimizing Variables in PARROT | 32 |
| POP-File Syntax | 17 | Creating the Workspace File | 33 |
| Entering Experimental Information | 18 | Compiling the POP-file | 33 |
| Creating a New Equilibrium | 19 | Returning Control to the Console ... | 34 |
| Setting Equilibrium Conditions and its Uncertainty | 19 | Optimizing in PARROT | 35 |
| Setting Reference States | 20 | Optimizing the System in PARROT ... | 36 |
| Entering the Experimental Value and its Uncertainty | 21 | Changes that Require POP-file Recompilation | 36 |
| Entering Many Equilibria as a Table | 22 | Optimization Workflow | 36 |
| Setting Site Fraction Start Values | 24 | Ensuring Computation of all Equilibria | 37 |
| Commenting About an Equilibrium | 24 | Setting Weights | 38 |
| Simultaneous Use of Binary and Ternary Experiments | 25 | Optimizing and Evaluating Results ... | 39 |
| Using Stability Conditions | 25 | The Critical Set of Experiments | 40 |
| | | Continuing the Optimization and | 40 |

| | |
|---------------------------------------------------------------|-----------|
| Resetting Variables | |
| Updating the Set of Optimizing Variables | 42 |
| Reducing the Number of Optimizing Variables | 43 |
| Plotting Intermediate Results | 43 |
| Superimposing Experimental Data from EXP-files | 44 |
| Finalizing the Optimization | 45 |
| Finishing the Optimization | 46 |
| Rounding off Optimizing Variable Values | 46 |
| Updating the Database File | 46 |
| Creating a Database File | 47 |
| Updating the Setup File and the POP-file | 47 |
| Alternate Mode | 48 |
| About Alternate Mode | 49 |
| Optimizing in Alternate Mode | 50 |
| Preparing the POP-file for Alternate Mode | 50 |
| Examples of SET_ALTERNATE_CONDITION | 50 |
| Entering Other Experiments in the POP with Alternate Mode .. | 51 |
| Troubleshooting | 53 |
| Useful Guidelines | 54 |
| GES5 and GES6 Calculation Engine Version | 55 |
| Excluding and Including the Correct Equilibria | 55 |
| Conflicting Data | 56 |
| Experiments and Experimental Data | 57 |
| Phase Diagram Data | 58 |
| Data for Individual Compounds | 59 |
| Single Phase Mixing Enthalpies or Partial Enthalpies | 60 |
| Enthalpies of Formation and Enthalpies of Reactions | 61 |
| Chemical Potentials via EMF Measurements | 61 |
| Driving Force for Metastable Phases | 62 |
| Pressure-Temperature-Volume EOS Data | 62 |
| Crystal Structure, Lattice Parameters and Site-Occupancy | 63 |
| Magnetism and Other Atomistic Properties | 63 |
| Data About Systems of Different Orders | 64 |
| Thermodynamic Models | 65 |
| Gas | 66 |
| Compound Energy Formalism | 66 |
| Substitutional Liquid | 67 |
| Ionic Two-Sublattice Liquid Model .. | 67 |
| Models for Ordered Phases | 68 |
| 4SL Model for FCC, HCP and BCC ... | 69 |

| | |
|-------------------------------------------------------------|----------|
| 2SL Model for FCC, HCP and BCC ... | 70 |
| Magnetic Ordering | 71 |
| Molar Volumes and High Pressure .. | 71 |
| Excess Models | 72 |
| Database Manager User Guide | 1 |
| Introduction to the Database Manager Guide | 2 |
| Thermodynamic and Kinetic/Mobility Databases | 3 |
| Initialization of the TDB Module | 3 |
| The Database Definition File and Keywords | 5 |
| Database Definition File Syntax | 6 |
| ELEMENT | 7 |
| SPECIES | 8 |
| PHASE | 9 |
| Examples of Recommended Suffixes | 9 |
| GIBBS Phase-type Codes | 10 |
| Additional clarification | 11 |
| CONSTITUENT | 14 |
| ADD_CONSTITUENT | 15 |
| COMPOUND_PHASE | 16 |
| ALLOTROPIC_PHASE | 16 |
| TEMPERATURE_LIMITS | 17 |
| DEFINE_SYSTEM_DEFAULT | 17 |
| DEFAULT_COMMAND | 17 |
| DATABASE_INFORMATION | 18 |

| | |
|----------------------------------------------------------------------|-----------|
| TYPE_DEFINITION | 19 |
| FTP_FILE | 22 |
| FUNCTION | 23 |
| PARAMETER | 26 |
| GIBBS Parameter Name | 27 |
| Parameters for the Two Sublattice Ionic Liquid Model ... | 32 |
| OPTIONS | 33 |
| TABLE | 34 |
| ASSESSED_SYSTEMS | 35 |
| REFERENCE_FILE | 38 |
| LIST_OF_REFERENCE | 39 |
| ADD_REFERENCE | 40 |
| CASE and ENDCASE | 41 |
| VERSION_DATA | 42 |
| Working with the Mobility Databases | 43 |
| Extensions to Database Definition File Syntax | 44 |
| PARAMETER | 44 |
| DIFFUSION | 45 |
| ZEROVOLUME_SPECIES | 46 |
| Database Definition File Examples .. | 47 |
| Example 1: A Steel Database | 48 |
| Example 2: A Custom Database for the Sb-Sn Binary System | 49 |
| Example 3: A Public Database for the Fe-Cr-C Ternary System | 52 |

The Database Checker67

About the Database Checker68

Custom Databases: GES5 and
GES6 Calculation Engine
Version68

Database Checker Revision History 69

DATAPLOT User Guide 1**Introduction to the DATAPLOT User
Guide 2**

Using this Guide 3

About the DATAPLOT Graphical
Language 3

DATAPLOT Examples 4

Plotting Experimental Data Files 4

Graphical Mode 4

Console Mode 4

**Using DATAPLOT Graphical
Language 6**

DATAPLOT File Structure 7

DATAPLOT Language Syntax 7

Coordinate Systems 7

Graphical Operation Codes 8

Tables or Blocks 9

Drawing a Polygon10

Drawing an Analytical Function10

Painting of an Enclosed Area10

Writing a Text11

Plotting a Symbol11

Other Commands11

General11

ATTRIBUTE 12

CLIP 12

COLOR12

INCLUDE 12

LINETYPE12

Interactive Plotting12

Formatting DIGLAB Symbols in
LaTeX Documents 13

LaTeX Formatting Codes14

LTEXT vs LaTeX Commands for
Labels 15**PROLOGUE Commands16**

PROLOG 17

DIAGRAM_TYPE17

TIC_TYPE 17

TITLE17

XLENGTH 18

XSCALE18

XTEXT18

XTYPE18

YLENGTH 18

YSCALE18

YTEXT19

YTYPE19

DATASET Commands 20

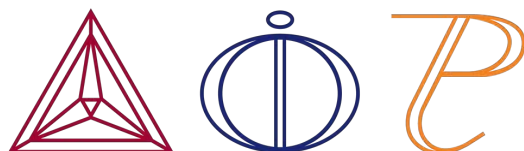
| | | | |
|-----------------------------------------------------|-----------|-------------------------------------------------------------|----|
| ATTRIBUTE | 21 | Example 2 – Draw Polygons and Symbols | 32 |
| BLOCK | 21 | Output Example | 32 |
| BLOCKEND | 22 | Macro Text | 33 |
| CHARSIZE | 22 | Example 3 – Using Strings and Various Line Types | 34 |
| CLIP | 22 | Output Example | 34 |
| COLOR | 23 | Macro Text | 34 |
| DATASET | 24 | Example 4 – Draw Curves Defined by Functions | 36 |
| DATAPOINT | 24 | Output Example | 37 |
| DRAWLINE | 24 | Macro Text | 37 |
| FONT | 25 | Example 5 – Use Included Files for Predefined Symbols | 38 |
| Font Numbers | 25 | Output Example | 38 |
| FUNCTION | 25 | Macro Text | 39 |
| GLOBALSIZE | 26 | Example 6 – Triangular Diagrams for Ternary Systems | 40 |
| INCLUDE | 26 | Output Example | 40 |
| LINETYPE | 26 | Macro Text | 41 |
| Line Types | 27 | Example 7 – Color Codes | 46 |
| PAINT | 27 | Output Example | 47 |
| PCFUNCTION | 27 | Macro Text | 47 |
| SYMBOLSIZE | 28 | Example 8 - DIGLIB Symbols | 51 |
| STRING | 28 | Output Example | 52 |
| TEXT | 29 | Macro Text | 52 |
| Examples of DATAPLOT Files and Outputs | 30 | Example 9 - DIGLIB Fonts and Lines | 59 |
| Example 1 – Draw Lines and Symbols | 31 | Output Example | 59 |
| Output Example | 31 | | |
| Macro Text | 31 | | |

| | |
|-------------------------------------------------------|-----------|
| Macro Text | 59 |
| Pourbaix Diagrams | 1 |
| Introduction to Pourbaix Diagrams .. | 2 |
| About Pourbaix Diagrams in Thermo-Calc | 3 |
| GES5 and GES6 Calculation Engine Version | 3 |
| Pourbaix Diagrams | 4 |
| Working with Pourbaix Diagrams ... | 6 |
| Key Concepts | 7 |
| Effective Interaction Ratio | 7 |
| Solubility | 8 |
| Basic Settings and Definitions | 9 |
| Thermodynamic Data Requirements | 11 |
| Required Thermodynamic Data | 12 |
| Including or Excluding the Gas Phase | 12 |
| Examples of Pourbaix Diagrams for Fe | 17 |
| Pourbaix Diagrams with Gas Phase Excluded | 18 |
| Pourbaix Diagrams with Gas Phase Included | 18 |
| Other Examples of Pourbaix Diagrams | 20 |
| Variations of Pourbaix Diagrams ... | 21 |
| Pourbaix Diagrams for Complex Alloys | 23 |
| Pourbaix Diagram References | 25 |

Installation Guide

Windows®, macOS® or Linux Operating Systems

Thermo-Calc Version 2020a



Installing Thermo-Calc

In this section:

| | |
|--------------------------------------------------------|---|
| Key to Using this Guide | 3 |
| Installation Terminology | 4 |
| About the Thermo-Calc Components To Be Installed | 6 |
| System Requirements and Platforms Tested | 7 |

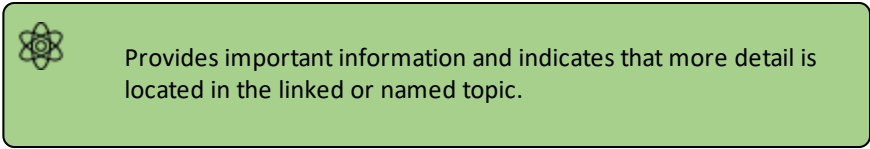



Key to Using this Guide

This installation guide is for all Thermo-Calc installations running on Windows, macOS or Linux operating systems. It is also applicable to demo (trial) installations as well as previously installed versions of Thermo-Calc (the new version is installed alongside the old version).

This guide includes information about:

- The types of licenses and installations available.
- Installing the Thermo-Calc software and its components on stand-alone computers, servers and client computers.
- Installing the license management software for network installations.
- Retrieving and installing license files.
- Troubleshooting to solve common installation problems.

ICONS IN THIS GUIDE

| Name | Description |
|--------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Information |  Provides important information and indicates that more detail is located in the linked or named topic. |
| Note |  The information can be of use to you. It is recommended that you read the text or follow the link. |
| Operating system | The operating system is indicated when the information is specific to a <i>Windows</i> , <i>macOS</i> or <i>Linux</i> operating system. |
|  License file | The license file, which contains the license keys and is installed on either a standalone computer or a network server. |
|  Thermo-Calc | The Thermo-Calc software and its components (including databases) to be installed. |

TYPOGRAPHICAL CONVENTIONS

| Convention | Definition |
|----------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Forward arrow → | The forward arrow symbol → instructs you to select a series of menu items in a specific order. For example, Tools → Options is equivalent to: From the Tools menu, select Options . |
| Boldface font | A boldface font indicates that the given word(s) are shown that way in on a toolbar button or as a menu selection. For example, if you are told to select a menu item in a particular order, such as Tools → Options , or to click Save . |
| <i>Italic</i> font | An <i>italic</i> font indicates the introduction of important terminology. Expect to find an explanation in the same paragraph or elsewhere in the guide. |
| <code>code</code> and <code>code bold</code> | A <code>code</code> font indicates you are to make a keyboard entry. It also shows a programming code or code examples. The <code>code bold</code> font highlights the entry. |

Installation Terminology

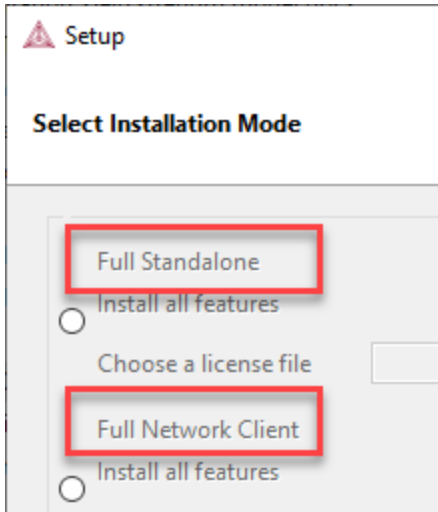
| Term | Definition |
|----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| client | A computer without a license file of its own but connected through the network to a computer with the license information. The client receives a license token from the computer where the license management software is installed. |
| consolidated network | A type of network installation where the Thermo-Calc software and a Thermo-Calc licensing software are installed on a single server computer. This allows all computers in the network to access both the software and a license on the server via a client installation. |
| distributed network | A type of network installation where the Thermo-Calc software is installed on one server computer in a network and the Thermo-Calc licensing software is installed on a different computer. After a thin client installation, all computers in the network can access both the software and the network license key via the server. |
| host ID | The MAC address on the computer that a license is locked to. |
| license file | The file (called <i>lservrc</i>) that contains all the purchased license keys. It is issued by Thermo-Calc Software, usually by email. |
| license key | The information contained in the license file that represents the products purchased and which is then authorised for installation. |

| Term | Definition |
|-----------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| License Manager (Windows) | The Windows program used for license management: it distributes license tokens as specified in the network license file issued by Thermo-Calc Software. |
| License Server (Linux) | The Linux program used for license management: it distributes license tokens as specified in the network license file issued by Thermo-Calc Software. |
| license server | The use of the term <i>license server</i> (lower case letters) is reserved for use for scripts and option files (for example, in an "Unattended Network Client Installations" on page 44). For the purposes of the step-by-step instructions it is not used to refer to the type of network installation that runs the license management program. Also see <i>License Manager</i> (Windows) and <i>License Server</i> (Linux). |
| licensing software | The Thermo-Calc license management software. When working in Windows it is called <i>License Manager</i> (full name is Sentinel RMS License Manager by SafeNet) and on Linux it is called <i>License Server</i> (full name is Sentinel License Sever by Safenet). |
| Network License (NWL) | <p>The license type used with the licensing software. The NWL can only be used on one specific computer that hosts the licensing software. This restricts license usage to a certain subnet or subnets.</p> <p>The software may be used on the number of sites you have paid for and by the number of persons you have paid for on any number of network connected computers</p> |
| standalone computer | A computer which uses a SUNLL license type. |
| Single-User-Node Locked-License (SUNLL) | A unique license file for one designated computer at one designated site. It cannot be copied or moved outside the site. If the software is installed on a portable computer, it can be temporarily used off-site. The license can be used without network access (to the License Server). |
| thin client | An installation where the software is installed on a file server but is run from a client computer. The licensing software may be installed on the file server (consolidated network installation) or on a different computer (distributed network installation). |
| XQuartz | An open-source X Windows System, which is required to run Thermo-Calc on a Mac. |

About the Thermo-Calc Components To Be Installed

What is installed with a Full Standalone or Full Network Client Option?

At the start of the installation process, the following components are installed when you choose either the **Full Standalone** or **Full Network Client** options. If you want to exclude a component (perhaps one of the SDKs), then you would use the **Custom** option.



A full installation means that all listed feature components are installed but the availability of the individual components is based on the license you have. This is also applicable to the databases and software development kits (SDKs).

Thermo-Calc

The Thermo-Calc software includes several add-on features and capabilities that are packaged with the software and included with a full standalone or network client installation. For example, there are the specialized add-on products Diffusion Module (DICTRA), Precipitation Module (TC-PRISMA), and Process Metallurgy Module as well as the Steel Model Library. For most of these specialized features, demonstration (*demo*) versions and examples area available for all users but advanced features are only available with a license.

Databases

All the latest databases are installed. As with the software features, availability of a specific database in the software itself is based on license. However, several demonstration (*demo*) databases are included and available to all users.

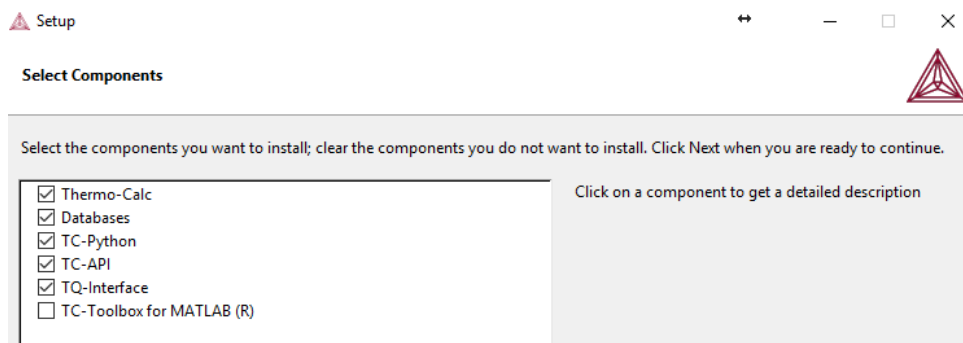
Software Development Kits (SDKs)

When the **Full Standalone** or **Full Network Client** option is chosen, it installs the TC-Python, TC-API and TQ-Interface SDKs. It does not install TC-Toolbox for MATLAB® (available only for Windows) unless the program finds a MATLAB® installation on your computer during this installation process, at which point you are asked if this component should be also be installed.

The TC-Python program is installed when the **Full Standalone** or **Full Network Client** option is chosen, but there are additional steps required to complete the installation as described separately in the *TC-Python Quick Installation Guide*.

What does the Custom option allow me to do during an installation?

During the installation process, there is some flexibility to choose what to include or exclude with the installation by choosing the **Custom** option. This is primarily to the level of being able to choose the SDKs or to exclude all databases or Thermo-Calc itself. That is, you cannot choose specific Thermo-Calc features or databases as these are controlled by the license and not the installation procedure.



System Requirements and Platforms Tested

► ["About the Thermo-Calc Components To Be Installed" on the previous page](#)

A full list of [system requirements](#) and program availability are found on the Thermo-Calc website. You can also see our [roadmap for platform support](#) to use for planning purposes. The software development kits (SDKs) are available as follows for the indicated platforms:

| SDK | Windows | Mac | Linux |
|-----------|---------|-----|-------|
| TC-Python | x | x | x |

| SDK | Windows | Mac | Linux |
|------------------------|---------|---------------|---------------|
| TQ-Interface | x | not available | x |
| TC-API | x | not available | x |
| TC-Toolbox for MATLAB® | x | not available | not available |

Thermo-Calc and its components are tested on these platforms for Thermo-Calc 2020a:

Platforms Tested by Operating System

| Windows | Mac | Linux ^{1, 2} |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------|-------------------------------------------------------------------------------------------------------------------------|
| Windows 10 64-bit | macOS X Catalina 10.15.1 | <ul style="list-style-type: none"> • Ubuntu 19.04 (Disco) • CentOS 7.6 • OpenSUSE 15.0 |
| <p>¹ Thermo-Calc Software cannot guarantee full functionality if the software is installed on other Linux distributions.</p> <p>² If you are installing on CentOS 7, it is recommended you install gtk2 before you run the installation script.</p> | | |

License and Installation Types

In this section:

| | |
|----------------------------------------------|----|
| License and Installation Types | 10 |
| About License Keys and Files | 10 |
| Standalone Installations (SUNLL) | 11 |
| Multi-User Network Installations (NWL) | 11 |

License and Installation Types

Installation procedures are based on the license type, the installation type and the operating system.



Demo (trial) installations: Only a standalone installation is available and a license file is automatically installed.

| License type | Installation Type | Windows | macOS | Linux |
|--------------|-------------------------------------------|---------|------------------|-------|
| SUNLL | Standalone | Yes | Yes | Yes |
| NWL | Consolidated network | Yes | No | Yes |
| | Distributed network | Yes | No | Yes |
| | License installations on a server network | Yes | Yes ¹ | Yes |

¹ For macOS, the licensing software is installed on a Windows or Linux computer server.

► www.thermocalc.com/purchase/licensing-options/

About License Keys and Files



Demo (trial) installations: A license file is automatically installed with the software. You do not need to request it.



To run Thermo-Calc and its components you need a valid license key for each product. The license keys are included in the license file emailed to you by Thermo-Calc Software.

You can copy the license file to the applicable computer(s) before or after installing the software—the license file itself is not required during the installation process. However, it is required to make calculations in Thermo-Calc.

► ["Request a License File from Thermo-Calc Software" on page 47](#)

Standalone Installations (SUNLL)

The standalone installation is used with the Single-User Node-Locked License (SUNLL). The

Thermo-Calc software  and a Thermo-Calc license file  are installed on a standalone computer. You can do a full (all operating systems) or a custom installation (Windows and Linux only).



- ▶ To get started, go to ["First Steps of Installation" on page 15](#) and then ["Standalone Installations" on page 23](#).

Multi-User Network Installations (NWL)

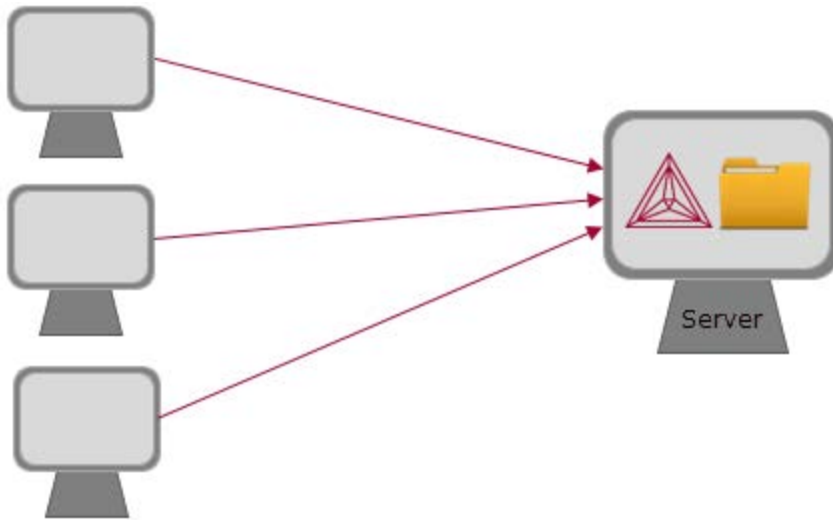
There are different types of multi-user network installations: consolidated, distributed and where the licensing software is installed on a computer network. There is also a subtype of installation called thin client, which is a step done with the consolidated and distributed network installations.





Thin client installations: A thin client installation is where the Thermo-Calc software is installed on a computer server but is run from a client computer. The licensing software can be installed on the computer server (a consolidated network) or on a different computer (a distributed network). This type of installation is available for Windows and Linux operating systems. The client computer must have the Thermo-Calc software installed. This type of installation mainly sets environmental variables and paths on the client computer.

Consolidated Network Installations

The consolidated network installation is used with a Network License (NWL) and it is available for Windows and Linux operating systems.

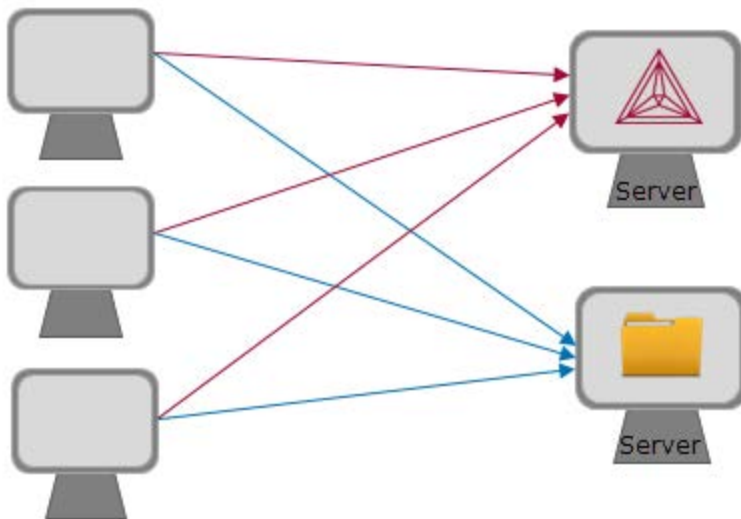




The Thermo-Calc software  and the license management program are installed on the same server where the license file  is also copied. A thin client installation allows all computers (the clients) in the server network to access both the software and the licensing on the same computer server.

- ▶ To get started, go to ["First Steps of Installation" on page 15](#) and then ["Network Client Installations" on page 32](#).

Distributed Network Installations

The distributed network installation is used with a Network License (NWL) and is available for Windows and Linux operating systems.

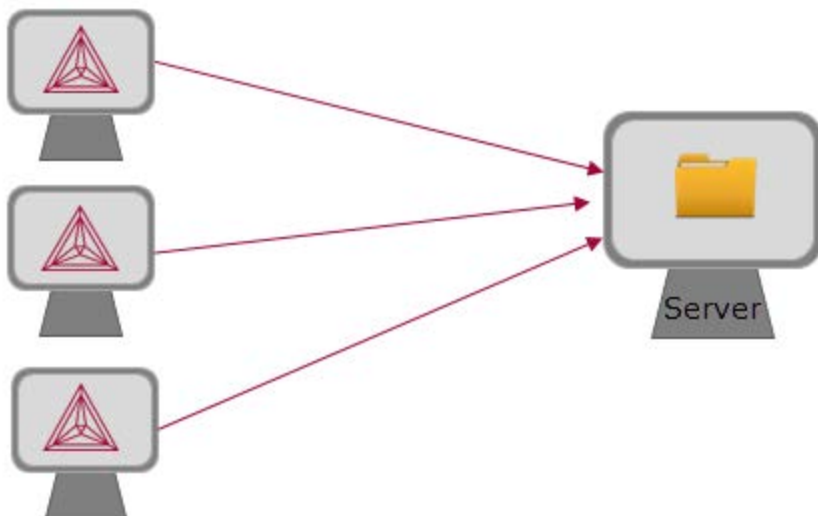




The Thermo-Calc software  is installed on one computer server in a network and the licensing software is installed on a different computer server where the license file  is also copied. A thin client installation allows all computers (the clients) in the server network to access both the software and the licensing on the two computer servers.

- ▶ To get started, go to ["First Steps of Installation" on page 15](#) and then ["Network Client Installations" on page 32](#).

License Installations on a Server Network

When a license file is installed on a server network, it is used with a Network License (NWL). It is available for all platforms. However, for macOS the server containing the licensing software must be set up on Windows or Linux.



The licensing software is installed on a computer server where the license file  is also copied. The Thermo-Calc software  is installed on every computer in the network that needs it.

- ▶ To get started, go to ["First Steps of Installation" on page 15](#) and then ["Network Client Installations" on page 32](#).

Preparing for Installation

In this section:

| | |
|------------------------------------------------|----|
| First Steps of Installation | 15 |
| Default Directory Installation Locations | 15 |
| Subnet Information for Network Licenses | 20 |
| macOS Installation Notes | 21 |
| Linux Installation Notes | 22 |

First Steps of Installation

This section reviews some of the things you need to do before installing the Thermo-Calc software.

- Learn about the default directories where the software and license files are installed.
- For network installations, collect subnet information.
- For Mac, install XQuartz and make sure the security preferences are set correctly.
- For a Linux Cent OS 7 installation, also install gtk2 before you run the installation script.

```
yum install gtk2
```



Should I get my license file before or after software installation? The license file itself is not required during the installation process (and not at all for demo installations). However, it is required to make calculations in Thermo-Calc. The license file has details about your computer(s) that in some cases cannot be determined accurately until *after* installation (especially for a network installation). For most users it is recommended you request the file before you start installing.

Default Directory Installation Locations

The default directories where the software and its components are installed, including where the license file is stored, vary by platform and user type.




If you want to select specific components to install or if you want to install the software in a non-default installation directory, then do a custom installation (Windows and Linux only). In the table, <user> stands for the user name and <version> for the version of Thermo-Calc, for example 2020a.

Thermo-Calc Default Directory Locations








LICENSE FILE - ALL OPERATING SYSTEMS

The license file is installed outside of the installation program folder. If you have more than one version of Thermo-Calc installed then there will be additional folders here and one license file.

On a Mac the license file is put in /Users/Shared/Thermo-Calc. The example below is for a Standalone Windows installation.

| > This PC > OS (C:) > Program Files > Thermo-Calc > | | |
|-------------------------------------------------------------------------------------------|------------------|-------------|
| Name | Date modified | Type |
|  2019b | 2019-09-24 04:55 | File folder |
|  2020a | 2019-11-04 06:27 | File folder |
|  lservrc | 2019-09-24 04:52 | File |

WINDOWS

| Windows user type | Default directory |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Administrator | <p>The Thermo-Calc program is installed here:</p> <p>Program Files\Thermo-Calc\<version></p> <p>The documents, materials, examples and other folders that sometimes require additional licenses are installed here:</p> <p>C:\Users\Public\Public Documents\Thermo-Calc\<version></p> <div> <p>Name</p> <ul style="list-style-type: none">  Examples  Manuals  Materials  ProcessMetallurgyMaterials  PropertyModels  SDK </div> <p>A copy of the documents, materials, examples and more are then placed here:</p> <p>C:\Users\<user>\Documents\Thermo-Calc\<version></p> <div>  <p>It is recommended that you work with the files that are copied to the <i>user</i> folder.</p> </div> |
| License software installations on a server network (the License Manager software) | C:\Program Files (x86)\Common Files\SafeNet Sentinel\Sentinel RMS License Manager\WinNT\ |

MAC

| Mac user type | Default directory |
|-------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Administrator (user name and password required) | <p>The Thermo-Calc program is installed here in the Applications folder:</p> <p><code>Thermo-Calc-<version>.app</code>, <code>Thermo-Calc-<version>-Demo.app</code>, and, <code>uninstall-Thermo-Calc-<version>.app</code></p> <p>The documents, materials, examples and other folders that sometimes require additional licenses are installed here:</p> <p><code>/Users/Shared/Thermo-Calc/<version></code></p> <p>To go to this folder, in Finder, from the Go main menu select Go to folder. Enter the above file path and click Go.</p> |






LINUX

| Linux user type | Default directory |
|----------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Non root user | <p>The Thermo-Calc program including the documents, materials, examples and other folders that sometimes require additional licenses are installed here:</p> <p><code>/home/<user>/Thermo-Calc/<version></code></p> |
| Root user | <p>The Thermo-Calc program including the documents, materials, examples and other folders that sometimes require additional licenses are installed here:</p> <p><code>/opt/Thermo-Calc/<version></code></p> |
| License software installations on a server network (the License Server software) | <p>If you are doing a network installation then these files are available as a tar-file from the Thermo-Calc Software web site.</p> <p>In the downloaded tar-file, there is a restart_lserv script file, which can be used as a template for creating a script that starts up the License Server.</p> |

DATABASES

The standard Thermo-Calc databases and the database initialization file `tc_initd.tdb` are located in a subfolder to the Thermo-Calc installation. For example, in a Windows Standalone installation, you can find these in a folder called **data** where the file path is `C:\Program Files\Thermo-Calc\<version>\data`.

> This PC > OS (C:) > Program Files > Thermo-Calc > <version> > data

| Name | Type |
|-----------------------------------------------------------------------------------------------------------|----------------------|
|  tc_initd | Thermo-Calc TDB file |
|  STANDARD_DB_CLASSES.BIN | BIN File |
|  TCTI2 | File folder |
|  TCTI1 | File folder |
|  TCSLD3 | File folder |

TC-TOOLBOX FOR MATLAB

Examples for the TC-Toolbox are placed under MATLAB® in the same documents folder as the Thermo-Calc files (Documents folder):

```
..\Documents\MATLAB\Thermo-Calc-Toolbox-X\Examples
```

Where X is the installed version number of the toolbox.

For most installations the examples are available in the MATLAB window when the software is opened.

DATABASE CHECKER PROGRAM

The Thermo-Calc software package includes a program to check that the syntax of unencrypted database files is correct. The program applies the syntax rules set out in the *Database Manager User Guide* and reports errors and issues warnings. This program is intended for advanced users who develop and manage databases.



Thermo-Calc accepts deviations from these syntax rules. This means that a database can work even if the Database Checker reports errors and warnings. For example, an error is reported if an abbreviated phase name is found, but phase name abbreviations are accepted by Thermo-Calc and its add-on modules.

The executable **DatabaseChecker** file is found in the Thermo-Calc home directory. The program can also be launched by selecting **Tools→ Database Checker** from the main menu.

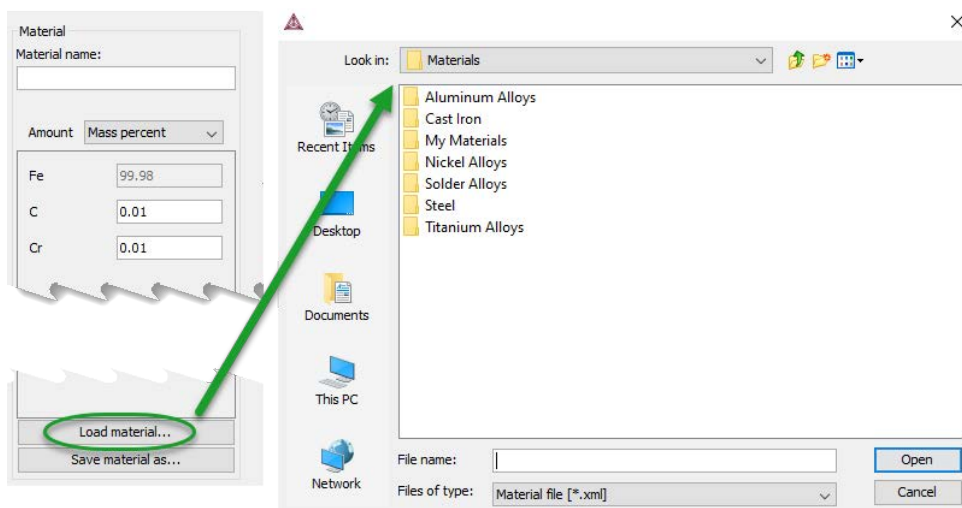
MATERIALS

When you are working with the System Definer you can open the default **Materials** folder included with your installation.

At the bottom of the window under **Material**, click **Load material** to navigate to a material file.



There is a separate folder for materials saved using the Process Metallurgy Calculator. See [Process Metallurgy Materials](#).



The default directory where these files are stored is based on operating system:

| Operating system | Materials installation directory |
|------------------|------------------------------------------------------------------------------------------------------------------------------------------------|
| Windows | C:\Users\<user>\Documents\Thermo-Calc\2020a\Materials |
| Linux | On Linux all user files are installed where the program is installed. If installed as root the default is: /opt/Thermo-Calc/2020a/Materials |
| Mac | /Users/Shared/Thermo-Calc/2020a/Materials |

CUSTOM PROPERTY MODELS



All property models (whether these are predefined or custom models) must be located in a subdirectory of the property model directory. You can go to **Tools**



→ **Options** and the **Model directory** field displays the default directory.

Predefined models included with the Property Model Calculator are installed in the locations below based on your operating system. If you create your own models, this is the default directory where these are saved. You can also use one of these as a template to create your own property model.

| Operating system | Property model installation directory |
|------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Windows | <code>C:\Users\<user>\Documents\Thermo-Calc\2020a\PropertyModels</code> |
| Linux | On Linux all user files are installed where the program is installed. If installed as root the default is: <code>/opt/Thermo-Calc/2020a/PropertyModels</code> |
| Mac | <code>/Users/Shared/Thermo-Calc/2020a/PropertyModels</code> |

PROCESS METALLURGY MATERIALS

With the Process Metallurgy Calculator you can save materials to work with again. This is the default folder where these are stored based on your operating system:

| Operating system | Process Metallurgy Materials installation directory |
|------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Windows | <code>C:\Users\<user>\Documents\Thermo-Calc\2020a\ProcessMetallurgyMaterials</code> |
| Linux | On Linux all user files are installed where the program is installed. If installed as root the default is: <code>/opt/Thermo-Calc/2020a/ProcessMetallurgyMaterials</code> |
| Mac | <code>/Users/Shared/Thermo-Calc/2020a/ProcessMetallurgyMaterials</code> |

Subnet Information for Network Licenses

For network licenses, the subnet information is also required. Ask your network administrator for the *network address for the subnet*. Additional requirements are included elsewhere for network installations.

-
- Subnets should be in the format aaa.bbb.ccc*** (for example: 192.168.29.0/24 or 192.168.29.*)
 - A maximum of six subnets are permitted.

An alternative way to get this information is to run the command:

- *Windows:* `ipconfig /all`
- *Mac/Linux:* `ip a`

macOS Installation Notes

RESTARTING AFTER AN INSTALLATION

In some types of installations (e.g. a network installation), you may have to restart your Mac to use Thermo-Calc for the first time.

INSTALLING XQUARTZ

The XQuartz open-source X Windows system is required to run Thermo-Calc on macOS X but it is not required to install Thermo-Calc. Before installing Thermo-Calc, you may also need to ensure that the computer security permissions are set.

1. In a web browser go to <https://www.macupdate.com> or to download it directly from XQuartz, <http://xquartz.macosforge.org/landing/>.
2. In the **Search Mac Apps** field, enter *XQuartz*.
3. Click the **XQuartz** search result. For example, based on the recent version, the name is XQuartz-2.7.7.dmg.
4. Click **Download**.
5. Double-click the **XQuartz.pkg** file. Follow the instructions.
6. Click **OK** when the message about logging out displays and click **Close** when the installation is successful.

ENABLING THE SECURITY SETTINGS

1. From the Apple main menu, select **System Preferences**.
2. Click **Security and Privacy**.
3. Click **General**. At the bottom of the **Security & Privacy** window, click the lock icon to

make changes. Enter the administrator password as required.

4. If you have already tried to launch the Thermo-Calc installer, you can click **Open Anyway** to proceed. Otherwise, under **Allow apps downloaded from:** click **Anywhere** and then **Allow from Anywhere**.
5. Continue with the applicable installation type (standalone or network).



Remember to reset your security after installing Thermo-Calc.

Linux Installation Notes

The following are details you need to know regarding your Linux installation as well as how to open Thermo-Calc.

openSUSE Administration (sudo) Users

Note the following if you are a sudo user (administrator) in openSUSE installing Thermo-Calc using this command:

```
sudo ./linux-installation-x64-6.0.0.17347.run
```

When this command is used, you will do a text-based installation instead of having a graphical interface to guide you. The information is the same, just without the user interface.

Opening Thermo-Calc in Linux

To open Thermo-Calc double-click the **Thermo-Calc-2020a** application or from the Thermo-Calc installation directory enter `$./Thermo-Calc-2020a.sh` in the terminal.

Standalone Installations

You can either do a full or a custom standalone installation. The license type is called a Single-User Node-Locked License (SUNLL).

In this section:

| | |
|------------------------------------------------------|----|
| Full Standalone Installations | 24 |
| Custom Standalone Installations | 27 |
| Add New Components to an Existing Installation | 30 |

Full Standalone Installations

The following describes a full standalone installation. These steps assume you have completed the section ["First Steps of Installation" on page 15](#).

Request your license file from Thermo-Calc Software



Demo (trial) installations: Skip this step. A license file is automatically installed with the software. You do not need to request it.



Updates to Thermo-Calc: Customers who subscribe to the annual maintenance plan can skip this step if you have received your license file in an email from Thermo-Calc Software AB. Save the license file to your computer to use during software installation. The license file name must be the same as the existing file name to ensure there are no errors during the update.

Follow the instructions for your operating system in the section ["Request a License File from Thermo-Calc Software" on page 47](#).

Download your Thermo-Calc installation software

- *Web downloads:* For web links sent in an email from Thermo-Calc Software, go to the URL and log in with the information provided to download the software.
- *DVD installations:* Insert the DVD and follow the instructions.

Run the applicable installation file for your operating system

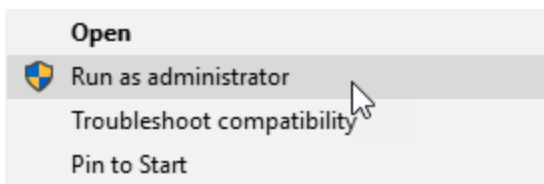
1. Navigate to the folder for your operating system and click the link to download the software package, then go to the folder where you downloaded it.



Administrative rights are required for Windows and Mac installations.

WINDOWS

Right-click the **.exe** file and choose **Run as administrator** to launch the **Setup** program.



MACOS

Double-click the downloaded file then follow the instructions.



For macOS and when you first run the installer, you may see a message that *Thermo-Calc-osx-<version> can't be opened because Apple cannot check it for malicious software*. If this happens, select **Show in Finder**. Then, in the opened **Finder** window right-click the downloaded file `Thermo-Calc-osx-<version>` and select **Open**.

LINUX

To start the Setup Wizard in a Terminal window, enter these commands in the directory where the installation file is saved:

```
> chmod +x linux-installation-x64-2020a.run  
> ./linux-installation-x64-2020a.run
```



If you are an openSUSE root user, see ["Linux Installation Notes" on page 22](#) for some information about your installation.

2. On the **Setup** window click **Next**.
3. On the **License Agreement** window click the button to accept the license agreement then click **Next**.



Demo (trial) installations: Your installation starts and is done when the **Completing the Thermo-Calc Demo Setup Wizard** opens. Click **Finish** and start using Thermo-Calc.

Select the installation type and upload the license file

► ["About the Thermo-Calc Components To Be Installed" on page 6](#)

1. In the **Select Installation Mode** window click **Full Standalone: Install all features**.




If you want to exclude a component (perhaps one of the SDKs), then you would use the **Custom** option. See ["Custom Standalone Installations" on the next page](#).

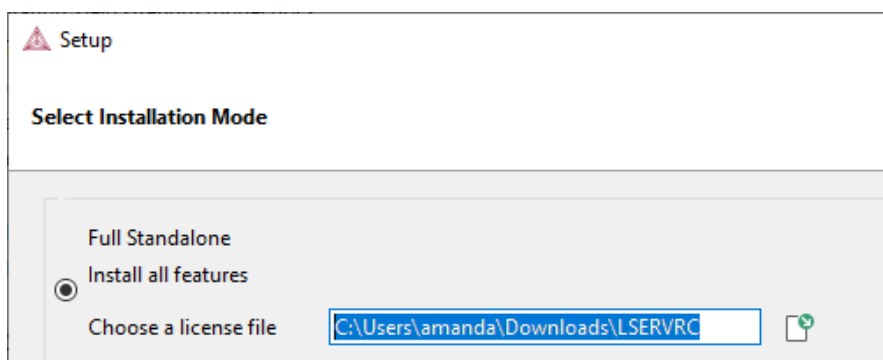


When the **Full Standalone** or **Full Network Client** option is chosen, it installs everything except the TC-Toolbox for MATLAB® (available for Windows only). However, if the program finds a MATLAB® installation on your computer during this installation process, you are prompted if this component should be also be installed.



The TC-Python program is installed when the **Full Standalone** or **Full Network Client** option is chosen, but there are additional steps required as described separately for this SDK.

2. For a **Full Standalone** installation, in the **Choose a license file** field either enter the file path or click the file button  to navigate to where you saved the license file emailed to you from Thermo-Calc Software. The license file is called **lservrc**. Click **Next**.





To prevent errors, leave this field blank if you did not get a license file yet.

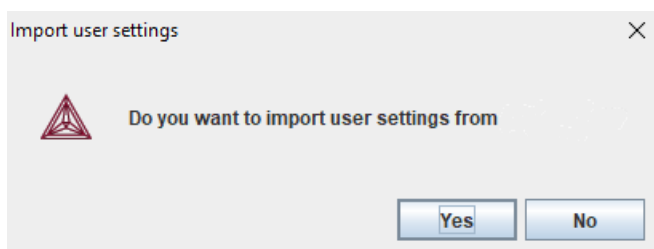
3. TC-Python is installed for all users even if you do not have a license. The **Install TC-Python** window is a reminder that additional installation procedures are required after Thermo-Calc is installed. Click **Next**.

Install the software and start using Thermo-Calc

1. In the **Ready to Install** window click **Next**.
2. Click **Finish** and start using Thermo-Calc. For Linux users, log out and log back in to finish the installation and start using Thermo-Calc.



macOS installations and if you have previous Thermo-Calc installations: When you launch Thermo-Calc with the new or updated version, the splash screen hides the **Import User Settings** dialog box. In order to proceed you need to click the splash screen and then click **Yes** or **No** in the dialog box.



- ▶ If you did not get your license file see ["Request a License File from Thermo-Calc Software" on page 47](#).

Custom Standalone Installations



["About the Thermo-Calc Components To Be Installed" on page 6](#)

Use the **Custom** option if you want more control over what component features to include or exclude, for example use it to exclude an SDK.

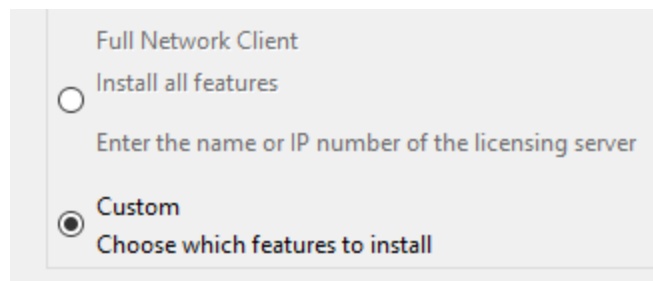
This topic describes how to do a custom installation on a standalone computer for either a Windows or Linux operating system. These steps assume you have completed these sections:

- ["First Steps of Installation" on page 15](#)
- Steps 1 to 3 of a ["Full Standalone Installations" on page 24](#) where you request your license file, download the software and then have started to set up the program up to the **Select Installation Mode** window.

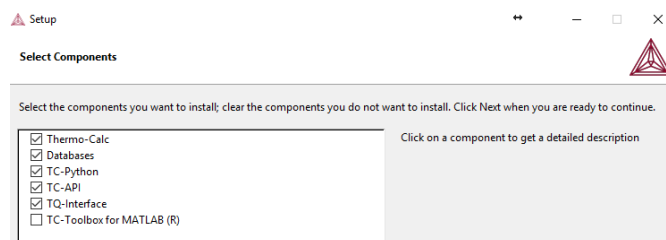
Select the installation mode and what components to include or exclude

["About the Thermo-Calc Components To Be Installed" on page 6](#)


1. In the **Select installation mode** window click **Custom** (the option appears greyed out, but it is available to select). Click **Next**.

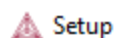


2. On the **Specify Configuration** window the **Create Shortcuts on Desktop** check box is selected by default. Click **Next**.
3. In the **Select Components** window, click to deselect the check boxes as needed. Click **Next**.



Set the installation directory and choose the license file

1. In the **Installation Directory** window, either accept the default path or enter a path to where you want to install the software (see ["Default Directory Installation Locations" on page 15](#)). Click the file button  to **Browse for Folder** and navigate to another directory. Click **Next**.



Installation Directory

Please specify the directory where Thermo-Calc will be installed.

Installation Directory




To prevent errors, leave this field blank if you do not have a license file yet.



For the Windows TC-Toolbox for MATLAB® component, and if you get a **MATLAB not found** message, enter the MATLAB® installation directory and click **Next**.

2. In the **Choose Setup Type** window, click **Standalone**.

The screenshot shows the 'Choose Setup Type' window. It has a title bar with a 'Setup' icon. Below the title bar is the section header 'Choose Setup Type'. The main area contains the text 'Select one of the following setup types. See installation guide for detailed description of the choices.' There are three radio buttons: 'Standalone' (selected), 'Choose a license file', and 'Network Client'. The 'Choose a license file' option has a text box containing 'C:\Users\amanda\Downloads\lserverc' and a file icon button. The 'Network Client' option has a text box for 'Enter name or IP number of the licensing server'.

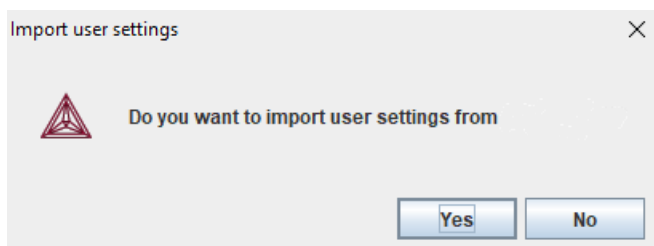
3. In the **Choose a license file** field enter the path to your license file (called **lserverc**) or click the file button  to navigate to a location on the computer and open the file. Click **Next**.
4. If **TC-Python** is selected to be installed, the **Install TC-Python** window is a reminder that additional installation procedures are required after Thermo-Calc is installed. Click **Next**.

Install the software and start using Thermo-Calc

1. In the **Ready to Install** window click **Next**.
2. Click **Finish** and start using Thermo-Calc. For Linux users, log out and log back in to finish the installation and start using Thermo-Calc.



macOS installations and if you have previous Thermo-Calc installations: When you launch Thermo-Calc with the new or updated version, the splash screen hides the **Import User Settings** dialog box. In order to proceed you need to click the splash screen and then click **Yes** or **No** in the dialog box.

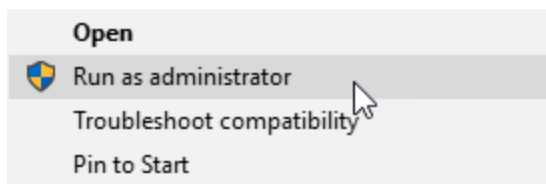


If you did not get your license file see ["Request a License File from Thermo-Calc Software" on page 47](#).

Add New Components to an Existing Installation

If you want to add new components to an existing Thermo-Calc installation (for example, you purchased a license for TC-Python), run the installation file again as in Step 3 of ["Full Standalone Installations" on page 24](#).

1. For all OS you need to have administrative level rights. For example in Windows, right-click the executable Thermo-Calc installation **.exe** file and choose **Run as administrator** to launch the **Setup** program.



2. Click **Next**. Click to accept the license agreement. Click **Next**.
3. Select the additional component(s) to install. Click **Next**.
4. Click **Next** to start the installation, which adds the new component(s).



Use the **Uninstall** program to *remove* components.



["Uninstalling Thermo-Calc" on page 65](#)

Network Client Installations

This installation type is available for all operating systems, however for macOS the License Server must be run on a Windows or Linux computer. It is applicable to the consolidated and distributed network types of installations as well as for the licensing installation on a server network.

▶ ["About the Thermo-Calc Components To Be Installed" on page 6](#)

In this section:

| | |
|-----------------------------------------------|----|
| Full Network Client Installations | 33 |
| Set Up the License Manager on Windows | 34 |
| Set Up the License Server on Linux | 36 |
| Thin Client Installations | 39 |
| Custom Network Client Installations | 41 |
| Unattended Network Client Installations | 44 |

Full Network Client Installations

The following outlines how you do a full network client installation.

Install the licensing software

Follow the instructions for your operating system:

- ["Set Up the License Manager on Windows" on the next page](#), or
- ["Set Up the License Server on Linux" on page 36](#)

Complete Steps 1 to 3 of a full standalone installation

These steps assume you have completed the instructions for ["Full Standalone Installations" on page 24](#) to download and run the software up to the **Select Installation Mode** window. It is up to you whether you get the computer information for the license files before or after installing the software.

Choose the installation type and enter the computer server details

► ["About the Thermo-Calc Components To Be Installed" on page 6](#)

1. In the **Select Installation Mode** window click **Full Network Client** to **Install all features** (the option appears greyed out, but it is available to select).



If you want to exclude a component (perhaps one of the SDKs), then use the **Custom** option and see ["Custom Network Client Installations" on page 41](#).

2. In the field, enter the name or IP number of the computer where the licensing software is installed. Click **Next**.

Full Network Client

☒ Install all features

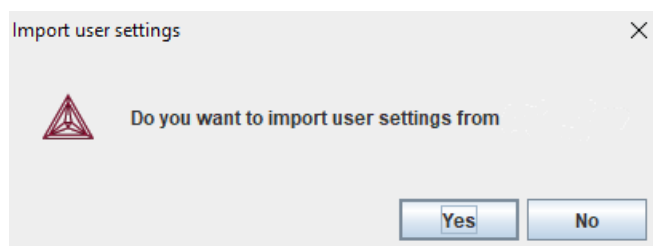
Enter the name or IP number of the licensing server

3. TC-Python is installed for all users even if you do not have a license. The **Install TC-Python** window is a reminder that additional installation procedures are required after Thermo-Calc is installed. Click **Next**.

4. In the **Ready to Install** window click **Next**.
5. When the **Completing the Thermo-Calc Setup Wizard** window opens, click **Finish**. For *Linux* users, log out and log back in to start using Thermo-Calc.



macOS installations and if you have previous Thermo-Calc installations: When you launch Thermo-Calc with the new or updated version, the splash screen hides the **Import User Settings** dialog box. In order to proceed you need to click the splash screen and then click **Yes** or **No** in the dialog box.



- ▶ If you did not get your license file see ["Request a License File from Thermo-Calc Software" on page 47](#).

Set Up the License Manager on Windows



License Manager vs License Server: Both terms refer to the licensing software program installed on a network computer. License Manger is for Windows and License Server is for Linux. See ["Installation Terminology" on page 4](#) for more information.

Installation Requirements

This procedure explains how to install the License Manager on a computer that acts as a license server in your network. It is a Sentinel RMS License Manager Windows service and it supplies the client computers in your network with license tokens when it runs the Thermo-Calc software. A network license can only be used on one specific computer that hosts the License Manager. The network license determines which client computers receive license tokens using their IP addresses and IP ranges.

- For *Mac* installations, the server containing the license file must be set up on a Windows or Linux computer.

-
- For testing purposes, and in order to confirm the installation is working correctly, install the Thermo-Calc software on the same computer as the Sentinel RMS License Manager. Thermo-Calc can always be uninstalled after testing if required.
 - Administrator rights are required.

Installing the License Manager on Windows

Install the Sentinel RMS License Manager software

1. Follow the instructions to [download your Thermo-Calc installation software](#).
2. Open the directory for Windows and right-click the file **Sentinel RMS License Manager 8.5.1.msi**.
3. Select **Save target as** and choose a suitable directory so that you can easily find the file later.
4. Right-click the downloaded file and choose **Install**. Click **Next**.

Choose the installation directory

1. Click to accept the license agreement. Click **Next**.
2. Enter your **User Name** and **Organization** and select to install the License Manager for **All users**. Click **Next**.
3. In the **Destination Folder** window click **Next** to accept the suggested destination directory or **Change** to select another directory. Click **Next**.

Choose the setup type and install the software

1. In the **Setup Type** window, select **Complete**. Click **Next**.
2. Select the **Unblock the system firewall for the Sentinel RMS License Manager** check box.



Selecting the check box is required to run Thermo-Calc.

3. Click **Next** and then **Install**.
4. Click **Finish** to exit the InstallShield Wizard.

Copy the license files to the destination directory

1. Copy the network license file to the destination directory. By default, it is installed in the following directory with the name **lservrc**.

```
C:\Program Files (x86)\Common Files\SafeNet  
Sentinel\Sentinel RMS License Manager\WinNT\
```



The name of the **license file** must be in lower case letters (**lservrc**). This is especially important if both Windows and Linux operating systems are part of your network; Linux commands and operations are case-sensitive.

If the default file path does not work, you can set the environmental variable **LSERVOPTS** to select the license file:

- a. In the Windows **Control Panel**, go to **System → Advanced system settings**.
- b. In **System Properties** select **Advanced → Environment Variables → New**.
- c. Enter the **Variable name** **LSERVOPTS** to specify the parameters with which the License Manager is started.
- d. To specify the path to the license file in the **Variable value** field enter the following and include the complete license file path and name.

```
-s <license file path and name>
```

Reboot or restart the license manager

Set Up the License Server on Linux



License Manager vs License Server: Both terms refer to the licensing software program installed on a network computer. License Manger is for Windows and License Server is for Linux. See ["Installation Terminology" on page 4](#) for more information.

Installation Requirements

There are a variety of things needed to prepare for a Linux License Server installation. The following points are described in this section.

- You need to stop older versions of the License Server before running the new one. To stop the license server you run **lsrvdown** .
- Root access to your computer is required or you need to be on the **sudoers** list.
- To run the License Server on a Linux 64-bit computer, you need to install 32-bit library support. For example, on CentOS this can be done by running the command:

```
>yum install glib2.i686
```

- You need a valid **lservrc** network license file supplied by Thermo-Calc Software and the actual License Server—a file(program) called **lserv**.



The name of the **license file** must be in lower case letters (**lservrc**) because Linux commands and operations are case-sensitive.

- The license file need to be read and writable by the license server(license manager)
- If you have a license server; Upgrade your license server if the new one is a higher version than the present one. Clients work with newer license servers(managers) but not necessarily with ones older than client.

OPENSUSE ADMINISTRATION (SUDO) USERS

Note the following if you are a sudo user (administrator) in openSUSE installing Thermo-Calc using this command:

```
sudo ./linux-installation-x64-6.0.0.17347.run
```

When this command is used, you will do a text-based installation instead of having a graphical interface to guide you. The information is the same, just without the user interface.

Installing the License Server on Linux

Stop any older versions of the License Server



Skip this step if this is a new installation.

1. To stop an old version of the License Server that is already running, go to the directory where the old file is found, and enter the commands:

```
>chmod +x <lsrvdown>
>./lsrvdown <host_name>
```

2. Edit existing scripts that start the older version of the License Server so that they start the newer version instead.



For more information about the **lservdown** utility, go to <http://sentinelrms.safenet-inc.com/RMSDocumentation/SysAdmin/Content/lsrvdown.htm>

Write a script to start the License Server

The following is an excerpt from the template script for starting the License Server found in the `restart_lserv` file.

Replace the paths for `LICENSE_SERVER_DIR`, `LICENSE_FILE_DIR` and `LOG_DIR` to match your system. Save it as a script:

```
# set the directory where the executables are located
LICENSE_SERVER_DIR=/usr/local/Thermo-Calc/2020a/Licensing-files
# set the directory of the license file lservrc
LICENSE_FILE_DIR=/usr/local/Thermo-Calc/2020a/Licensing-files
# set the directory where you wish to save the log-files
LOG_DIR=/tmp
# stop the running server
# (omit this line if calling this script at startup)
$LICENSE_SERVER_DIR/lsrvdown $HOSTNAME
# start the license server
$LICENSE_SERVER_DIR/lserv -s $LICENSE_FILE_DIR/lservrc -l $LOG_DIR/lserv_use.log -f
$LOG_DIR/lserv_err.log
```

Confirm the HOSTNAME variable and open the UDP port

The hostname should always correspond to the DNS record verify this by doing the following.

1. Before starting the License Server make sure that the value of the `$HOSTNAME` variable is correct. This value can be shown by typing the `> nslookup $HOSTNAME` command in the terminal window:

The value should be the same IP address that is shown when you use the `ifconfig` command.

2. Open the UDP port 5093 in your firewall. In case you have installed SELinux you might also need to disable it by setting `SELINUX=permissive` in the `/etc/selinux/config` file.

Start the License Server

1. To start the License Server, run the script created as root. Enter these commands in the console:

```
> chmod +x <name_of_script_file>
> ./<name_of_script_file>
```

2. If you want the License Server to start when you boot the system, put a copy of the start script under `/etc/rc.d/init.d` and start the script from the file `/etc/rc.d/rc.local`.

Thin Client Installations

This topic describes how you install a thin Thermo-Calc client to run Thermo-Calc from a file server. It is applicable to consolidated and distributed network installations for either a Windows or Linux operating system.

INSTALLATION REQUIREMENTS

- You need access to the directory where Thermo-Calc is installed on the file server.
- You need the IP number or name of the computer where the license file is installed.
- For *Linux* you may have to disable your firewall. If SELinux is installed, try disabling it by setting `SELINUX=permissive` in `/etc/selinux/config`.

INSTALLING A THIN CLIENT ON WINDOWS

1. Map the file server share as a network drive so that it gets an assigned drive letter (e.g. **E:**).
2. Open the `\Thermo-Calc\<version>\` directory on the file server, where *version* is the current version of the software.
3. Open the directory **Thin-client**. Double-click the `Thermo-Calc-client-windows-`

`<version>.exe` file.

4. Click to accept the terms of the license agreement. Click **Next**.
5. Enter the name or IP number of where the license file and the License Manager software is installed. Click **Next**.
6. By default the **Create Shortcuts on Desktop** check box is selected. Click **Next**.
7. In the **Ready to Install** window, click **Next**.
8. Click **Finish**. To start Thermo-Calc find the program on the server and start it from there.

INSTALLING A THIN CLIENT ON LINUX

1. Add the following to the `smb.conf` file, where `<user>` is your user name:

```
[public]
path=/home/<user>/Thermo_Calc/2020a
public=yes
writable=yes
comment=smb share
guest OK=yes
force user=<user>
```

2. From the client, mount the directory on the server computer that contains the Thermo-Calc server installation (by default, this directory is called **/Thermo-Calc/2020a**). How the directory is mounted depends on the Linux distribution being used as well as how the Thermo-Calc directory on the server computer is shared. Use the Linux command `mount`. For example:

```
> mkdir public
> sudo mount -t cifs //ip_number_server_computer/public ./public -o
user=<user>
```

3. Open the mounted directory on your computer, and run `client-install-linux-x64.run` or `client-install-linux-x86.run` in the **/Thin-client** directory.
4. If you do this from the terminal window, use the following to start the installation (assuming that the file server is a 64-bit computer):

```
> ./client-install-linux-x64.run
```

5. Click **Forward** and click to select the license agreement. Click **Forward**.

6. Enter the name or IP number of the License Server. Click **Forward**.
7. If you are installing as a non-root user, by default, the **Create Shortcuts on Desktop** check box is selected. Click **Forward**.
8. In the **Ready to Install** window click Forward.
9. Click **Finish**. Log out and log back in to start using Thermo-Calc.

Custom Network Client Installations

This installation type is available for all operating systems, however for macOS the License Server must be run on a Windows or Linux computer. The requirements are the same as for a full client installation.

Install the licensing software

Follow the instructions for your operating system:

- ["Set Up the License Manager on Windows" on page 34](#), or
- ["Set Up the License Server on Linux" on page 36](#)

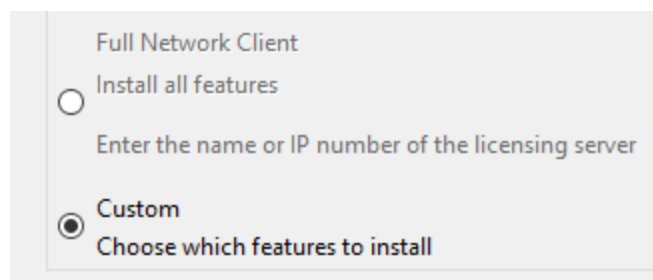
Complete Steps 1 to 4 of a full standalone installation

Follow the instructions for ["Full Standalone Installations" on page 24](#) to download and run the software. It is up to you whether you get the computer information for the license files before or after installing the software.

Select the installation mode and what components to include or exclude

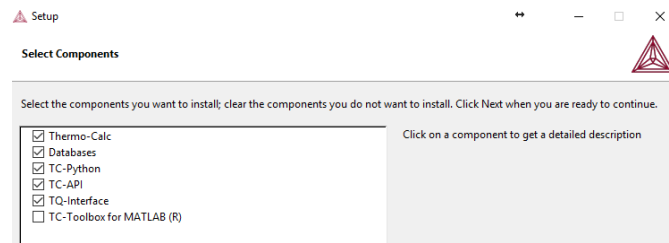
- ["About the Thermo-Calc Components To Be Installed" on page 6](#)

1. In the **Select installation mode** window click **Custom** (the option appears greyed out, but it is available to select). Click **Next**.




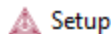
2. On the **Specify Configuration** window the **Create Shortcuts on Desktop** check box is selected by default. Click **Next**.

3. In the **Select Components** window, click to deselect the check boxes as needed. Click **Next**.

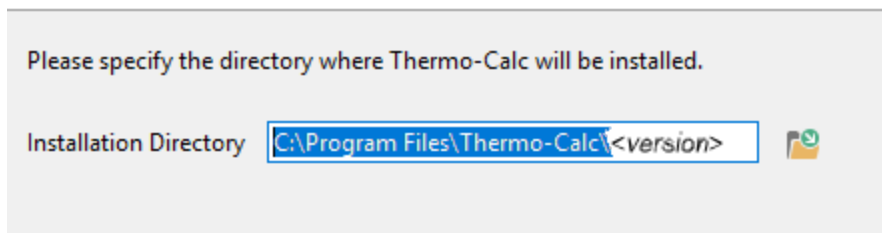


Set the installation directory and the file path to the license

1. In the **Installation Directory** window, either accept the default path or enter a path to where you want to install the software (see "[Default Directory Installation Locations](#)" on page 15). Click the file button  to **Browse for Folder** and navigate to another directory. Click **Next**.



Installation Directory

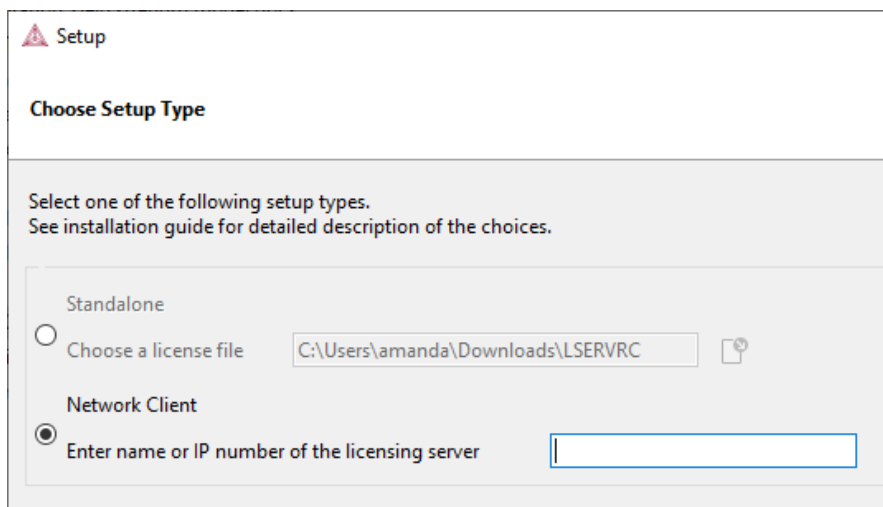


To prevent errors, leave this field blank if you do not have a license file yet.



For the Windows TC-Toolbox for MATLAB component and if you get a **MATLAB not found** message, enter the MATLAB® installation directory and click **Next**.

2. In the **Choose Setup Type** window, click **Network Client** and enter the name or IP number of the computer where the licensing software is installed. Click **Next**.



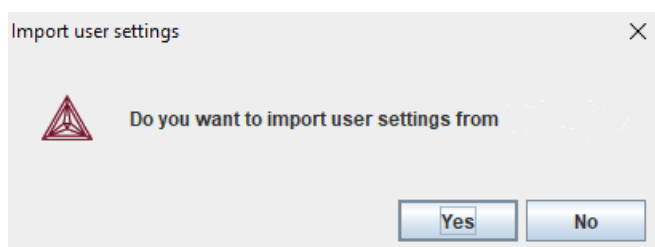
If you have selected to install **TC-Python** there is a reminder window that additional installation procedures are required after Thermo-Calc is installed. Click **Next**.

Install the software and start using Thermo-Calc

1. In the **Ready to Install** window click **Next**.
2. Click **Finish** and start using Thermo-Calc. For Linux users, log out and log back in to finish the installation and start using Thermo-Calc.



macOS installations and if you have previous Thermo-Calc installations: When you launch Thermo-Calc with the new or updated version, the splash screen hides the **Import User Settings** dialog box. In order to proceed you need to click the splash screen and then click **Yes** or **No** in the dialog box.



If you did not get your license file see ["Request a License File from Thermo-Calc Software" on page 47](#).

Unattended Network Client Installations



Terminology note: The use of the term *license server* (lower case letters) is applicable to the option files as described in this section. For the purposes of the step-by-step instructions it is not used to refer to the type of network installation that runs the licensing software.

Sometimes it is convenient to install Thermo-Calc network clients without providing user input after the installation is initiated (an unattended network client installation). This is available for Windows and Linux operating systems.



Make sure you know the name or IP number of the computer where the licensing software and the license file are to be installed.

Create an option file in a text editor to enter the options

The following is an example of an option file for a custom network client installation, where *<name/IP number>* is the name or IP number of the computer where the license file is installed:

```
installation_mode=custom
setup_type=client
enable-components=thermo,databases,tq,tcapi,toolbox,tcpython
icons=1
license_server=<name/IP number>
```

Below is a shorter example, specifying that a full Thermo-Calc network client should be installed:

```
installation_mode=full_client
license_server=<name/IP number>
```

Go to the directory where the installation file is stored



Thermo-Calc can only be installed in unattended mode from the command line prompt.

Start the installation in unattended mode using the option file created with this command:

- **For Windows:** `<installationfile>.exe --mode unattended --optionfile <path\optionfile>`

-
- For *Linux*: `<installationfile>.run --mode unattended --optionfile <path/optionfile>`

To see other options when you start the Thermo-Calc installation program from the command line prompt, run this command:

- For *Windows*: `<installationfile>.exe --help`
- For *Linux*: `<installationfile>.run --help`

Request License Files

In this section:

| | |
|--------------------------------------------------------|----|
| Request a License File from Thermo-Calc Software | 47 |
| Getting License Information Using Thermo-Calc | 47 |
| Requesting the License File for Windows or Linux | 48 |
| Requesting the License File for macOS | 50 |

Request a License File from Thermo-Calc Software

The following explains how to retrieve the necessary diagnostic and network adaptor information about your computer and then send an email to Thermo-Calc Software to get your license file(s) containing the license key(s).

To set up the correct licensing (excluding demo installations where a license file is not required):

1. Make a note of your company or organization's *site number*. You can find the site number on an invoice or any correspondence from Thermo-Calc Software.
2. Retrieve your computer diagnostic and network adapter information.
3. Email Thermo-Calc Software with this information.
4. A Thermo-Calc Software representative emails you the license file. Save the license file **lservrc** (there is no file suffix) to a location where you can easily access it later.

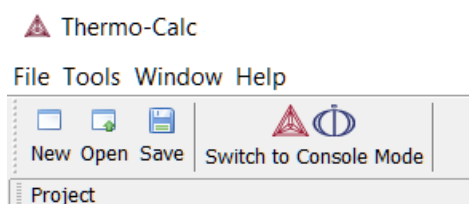
► <https://www.thermocalc.com/support/request-support/>

Getting License Information Using Thermo-Calc

If you have already installed Thermo-Calc, you can view the license information in the GUI. Select **Help → Show License Info**.

In Console Mode you can run the SYS module command `DISPLAY_LICENSE_INFO`.

1. Open Thermo-Calc.
2. Click **Switch to Console Mode**.



3. At the `SYS :` prompt, enter `DISPLAY_LICENSE_INFO` (all caps).



```
Thermo-Calc / DICTRA  
Only for use at Thermo-Calc Software AB  
Local contact Computer: orion.thermocalc.se
```

```
SYS:DISPLAY_LICENSE_INFO
```

4. You can output the information to a `FILE` or to the `SCREEN`.

```
SYS:DISPLAY_LICENSE_INFO  
OUTPUT TO SCREEN OR FILE /SCREEN/:SCREEN
```

5. For both options, the information is displayed on screen. Copy the section containing the **Ethernet** and **IP address**. You can save it to a text file or paste it directly into an email. If you choose `FILE` as the output, then you can attach the file to an email.

Requesting the License File for Windows or Linux

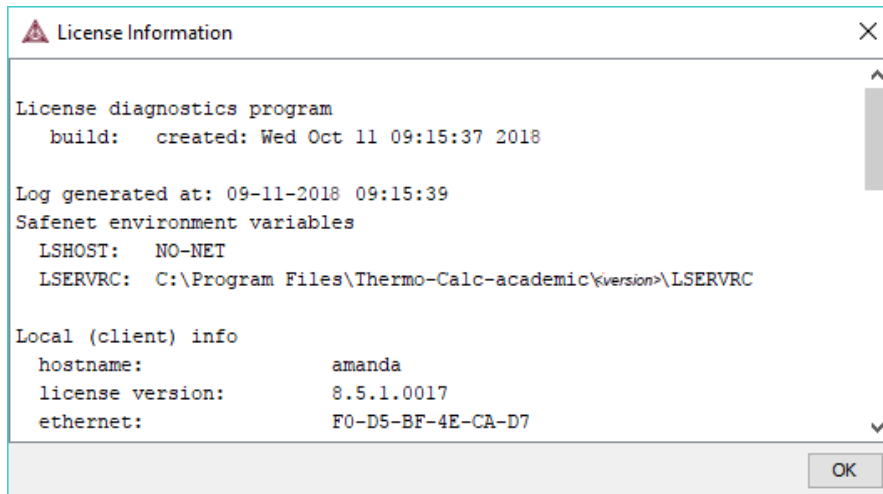


Demo (trial) installations: Skip this section. A license file is automatically installed with the software. You do not need to request it.



Upgrades to a new version of Thermo-Calc: Skip this section if you are upgrading to a new version of Thermo-Calc and (and you have a maintenance plan). Your license is sent to you in an email from Thermo-Calc Software AB. Save it to your computer to use during software installation.

1. To access the computer information you need to provide to get a license, start Thermo-Calc and select **Help → Show License Info**.



2. Copy the information from the **License Information** window. A lot of information may be shown below the initial screen, so make sure you scroll down to the end when you select and copy the window's contents. (Alternatively, you can copy the same information from the console by using the SYS module command DISPLAY_LICENSE_INFO.)
3. Send an email to support@thermocalc.com. Make sure to include the following in the subject line:

License diagnostic information from <Name> where Name is replaced with your **name**, the **organisation name** and the **Site Number**. *You can find the five-digit site number on an invoice or any correspondence from Thermo-Calc Software.*

Designated Site 12345
XYZ Company
Dpt. of Material Science
900 Main Street
Stockholm 11190
SWEDEN



4. A representative from Thermo-Calc Software replies to the email and attaches your license file(s).
5. Save the license file(s) to your computer or network.

Requesting the License File for macOS

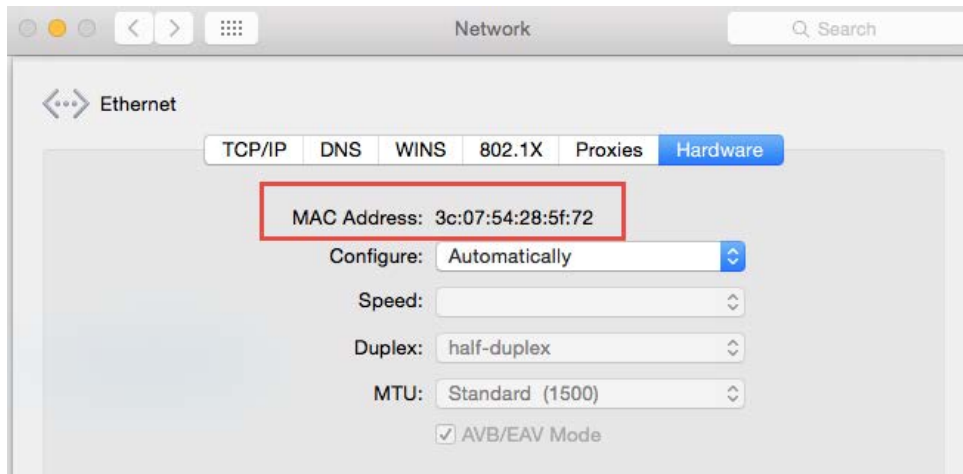


Demo (trial) installations: Skip this section. A license file is automatically installed with the software. You do not need to request it.



Upgrades to a new version of Thermo-Calc: Skip this section if you are upgrading to a new version of Thermo-Calc and (and you have a maintenance plan). Your license is sent to you in an email from Thermo-Calc Software AB. Save it to your computer to use during software installation.


1. From the Apple main menu, select **System Preferences**.
2. Click **Network**.
3. In the left column select **Ethernet** or **Built-in Ethernet** (do not select a WiFi connection as a local static MAC address is required).
4. Click **Advanced** → **Hardware**.
The **Network** window shows you the **MAC Address**. For example, the MAC address (the host ID) might be **3c:07:54:28:5f:72**.



5. Send an email to support@thermocalc.com and copy and paste the MAC address into the body of the email. Make sure to include the following in the subject line:

License diagnostic information from <Name> where Name is replaced with your **name**, the **organisation name** and the **Site Number**. *You can find the five-digit site number on an invoice or any correspondence from Thermo-Calc Software.*

Designated Site 12345
XYZ Company
Dpt. of Material Science
900 Main Street
Stockholm 11190
SWEDEN

| | |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------|
| To: | support@thermocalc.com |
| Cc: | |
| License diagnostic information from Jane Smith, XYZ Company, Site 12345 | |
| Add attachments  tclog.log (7.3 KB)  | |

6. A representative from Thermo-Calc Software replies to the email address provided and attaches your license file or files.
7. Save your license file to your computer or network.

Troubleshooting

In this section:

| | |
|----------------------------------------------------------------------|----|
| License Errors | 53 |
| Determining the Current License File Directory Path | 54 |
| Specifying a New Server Name or IP Number | 57 |
| MATLAB® Installation Directory | 58 |
| Firewalls | 59 |
| Client/Server Mismatch | 59 |
| macOS Installations: Running the License Initialization Script | 61 |
| Linux Installations: Running the License Initialization Script | 62 |

License Errors

| Issue | Platform | Installation type | Action or link to more information |
|-------------------------------------------------------------------------------------------------------------------|---------------|-------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| How do I add or update a standalone (SUNLL) license on a Windows computer where Thermo-Calc is already installed? | Windows | Standalone | "Determining the Current License File Directory Path" on the next page |
| How do I add or update a standalone (SUNLL) license on a Linux computer where Thermo-Calc is already installed? | Linux | Standalone | "Determining the Current License File Directory Path" on the next page |
| How do I add or update a network license on Windows? | Windows | Network | "Determining the Current License File Directory Path" on the next page |
| How do I add or update a network license on Linux? | Linux | Network | "Determining the Current License File Directory Path" on the next page |
| No license file found. Copy a valid license file to the installation directory after completing the installation. | All | All | You get this message if the wrong path or no license file is found at a path entered during the installation process. See "Default Directory Installation Locations" on page 15 and "Determining the Current License File Directory Path" on the next page |
| MATLAB® not found (for the TC-Toolbox for MATLAB component) | Windows | All | "MATLAB® Installation Directory " on page 58 |
| Warning Environment variable "LSHOST" is not set. Software will not function properly. | All | Network | "Specifying a New Server Name or IP Number" on page 57 |
| Problem running post-install step. Installation may not complete correctly. | Linux and Mac | Standalone | "macOS Installations: Running the License Initialization Script " on page 61 or "Linux Installations: Running the License Initialization Script" on page 62 |

| Issue | Platform | Installation type | Action or link to more information |
|---------------------------------------------------------------------------------------------------------------|-------------------|-------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Unable to run post-installation script, run the license initialization script as root after the installation. | | | |
| Firewall warnings related to license management software (License Manager and License Server) | Windows and Linux | Network | "Firewalls" on page 59 |
| Client / Server naming mismatches | Windows and Linux | Network | "Client/Server Mismatch" on page 59 |
| InstallScript engine missing | Windows | Network | You are not notified if the InstallScript scripting engine is not installed. Install the ISScript.msi file and then run the downloaded file from Thermo-Calc again as described in "Set Up the License Manager on Windows" on page 34 |

Determining the Current License File Directory Path

This topic explains how to find out where your license file is installed, either by default or if a different directory was chosen for previously installed versions. For new installations, where you may not have had a license file when you installed Thermo-Calc (for example, you had a demo version), you can also use these instructions to determine the correct file path.

From Thermo-Calc

If you have already installed Thermo-Calc, you can view the path to the license file in the GUI. Select **Help → Show License Info**.

In Console Mode you can run the SYS module command `DISPLAY_LICENSE_INFO`.

WINDOWS STANDALONE INSTALLATIONS

How do I add or update a standalone (SUNLL) license on a Windows computer where

Thermo-Calc is already installed?

1. Unpack the .zip file that contains your standalone license and save the LSERVRC file on your computer. Find out where to place the new license file by opening a Command Prompt Window (cmd.exe) and type in the command line:

```
>set LSERVRC
```

2. Press **Enter**. The output from the command is the path to the license file (including the name of the license file). For example: if the output is

```
LSERVRC=C:\Users\<user>\Documents\Thermo-Calc\lservrc
```

then the new license file should be placed in C:\Program Files\Thermo-Calc\2020a\

LINUX STANDALONE INSTALLATIONS

How do I add or update a standalone (SUNLL) license on a Linux computer where Thermo-Calc is already installed?

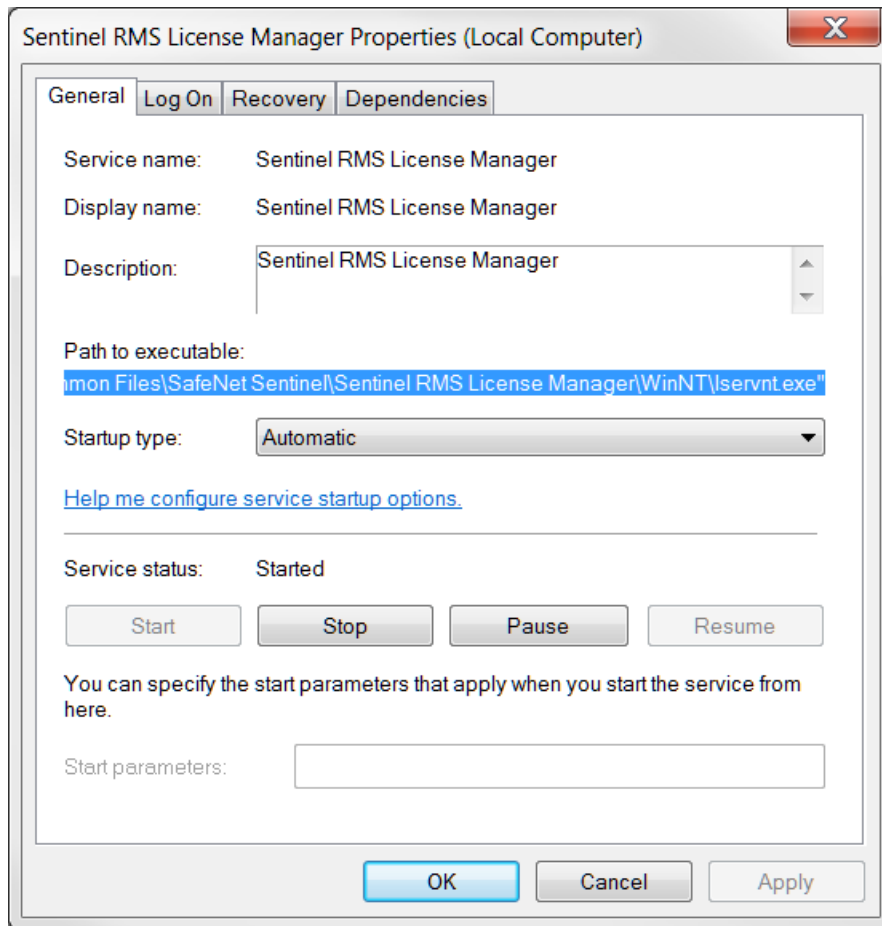
Find out where to place the new license file by opening a Terminal window and type in the command line:

```
echo $LSERVRC
```

WINDOWS NETWORK INSTALLATIONS

How do I add or update a network license on Windows?

1. You need administrator rights to do the following.
 - On *Windows 7*, click the Start button and in the search field type Services. Double-click the Services result.
 - On *Windows 8*, move the mouse over the right edge of the screen to access Search, click Settings and then enter and select View Local Services.
2. In the list of installed services, right-click **Sentinel RMS License Manager** and select **Properties** from the pop-up menu.
3. On the **General** tab under **Path to executable**, click the line containing the path to see where the file **lservnt.exe** is located. The license file (lservrc) is in the same directory.



The default path for the license file is

```
C:\Program Files (x86)\Common Files\SafeNet Sentinel\Sentinel RMS  
License Manager\WinNT\LSERVRC
```

4. Move your copy of the license file (lservrc) to this directory.
5. Restart the Sentinel RMS License Manager by:
 - Restarting the computer, or
 - Right-clicking **Sentinel RMS License Manager** and selecting **Restart** from the list of installed services.

LINUX NETWORK INSTALLATIONS

How do I add or update a network license on Linux?

Replace your current license file with the new license file. The license file is located in the same directory as the license server.

Specifying a New Server Name or IP Number

The Thermo-Calc Setup wizard does not warn you if the name or IP number entered to the server (with the license management software) is incorrect.

If the name or IP number is not set at all, or if it is set to an empty string, then when you start Thermo-Calc the following message displays: *Warning Environment variable "LSHOST" is not set. Software will not function properly.*

WINDOWS

This section explains how to specify or change the name or IP number of the server where the License Manager is installed and for a consolidated network client installation.

To install a license for an existing Thermo-Calc program, follow these steps:

1. Close all running Thermo-Calc programs.
2. Open a command line window.
3. Specify the name or IP number of the licensing software server. Type:

```
set LSHOST=<name/IP number>
```

To display the current name or IP number, type:

```
set LSHOST
```

MAC

Permanently set the environmental variable LSHOST to specify a new licensing server name or IP number. Refer to the file /Applications/Thermo-Calc-2020a.app/Contents/plist.info.

In this file, you can manually set the TC20A_HOME variable, which specifies the home directory of the Thermo-Calc program. See the plist.info file for an example.

LINUX

You can set or change the name or IP number of the license server at a later time by setting the environmental variable “LSHOST” to this name or number.

MATLAB® Installation Directory

For Windows installations of the TC-Toolbox for MATLAB® component, you may get an error message or window asking for the MATLAB installation directory path. If it is during the installation Setup process, enter the path in the field.

DETERMINING THE LICENSING SOFTWARE VERSION

Sometimes you may need to know the version of License Manager (Windows) or License Server (Linux) software being used. This can be useful while troubleshooting network installations.

-
- On *Windows* open a command prompt and go to the directory where `lservnt.exe` is found. For example:

```
>C:\Program Files (x86)\Common Files\SafeNet Sentinel\Sentinel RMS  
License Manager\WinNT
```

Type the command `>lservnt.exe -help` and the version is displayed.

- On *Linux* open a Terminal window and go to the directory where the `lserv` script is saved. For example:

```
>cd opt/Thermo-Calc/<version>/Licensing-files
```

Type the command `>./lserv -help` and the version is displayed.

Firewalls

WINDOWS

For a Windows License Manager installation you may have to change the system firewall settings to allow the License Manager to communicate with the computers running the client applications. Go to the Windows Firewall settings window to see if there are any problems. If prompted, select Unblock the system firewall for the Sentinel RMS License Manager and click Next.

LINUX

For a Linux License Server installation you need to open the UDP port 5093 in your firewall. In case you have installed SELinux you might also need to disable it by setting `SELINUX=permissive` in the `/etc/selinux/config` file.

Client/Server Mismatch

For some network installations there can be a naming mismatch that causes errors. The server (where the license management software is installed) gets information from its DNS servers that an IP address (`aaa.bbb.ccc`) belongs to a computer (Computer A). But the client computer identifies itself as having a different IP address (`aaa.bbb.ccc.eee`) for the same computer (Computer A).

Even if the IP address of the client computer belongs to a subnet range listed in the license file, there is a problem with accessing the license file because the computer name does not match the information.

You may need your organisation's network administrator to assist with this issue.

How to Check

Compare computer names on the client computer and server

1. On the client computer, start a command prompt **cmd.exe** and type `ipconfig /all`. Press `Enter`. A variety of data is displayed on screen. Write down the following information for later comparison:

- Hostname
- DNS Suffix
- Current IPv 4 Address

2. In the command window, type `nslookup <client_computer_name>`, where *client_computer_name* is the actual name of the client. Press `Enter`.

This shows what information is saved on the DNS Servers used by the client computer. This information should match what is shown in the output from the first step.

3. On the server that holds the license management software, open a command prompt and run the command line: `nslookup client_computer_name`. The output lists the information for this server.

Does it match the information given by the command `ipconfig /all` on the client computer? If not try the following:

Try these options to correct the issue

1. If the client computer has a dynamic (DHCP) IP address, either change it to a static one or make a reservation on the DHCP Server so that the computer always get the same IP address.
2. Update the records on the DNS Servers used by both the client computer and the server computer.

You can also configure the computer names and IP addresses in the local Hostfile of the client and server:

1. On the client computer, make a backup copy of the file `C:\Windows\System32\drivers\etc\hosts`.
2. Open the original in a simple text editor.
3. Add a new line which contains the IP and name of the server, for example:

-
- 192.168.29.27 license_server.thermocalc.se.
4. Save the changes.
 5. On the server, make a backup copy of the file `/etc/hosts`.
 6. Open the original in a simple text editor.
 7. Add a new line which contains the IP and name of the client, for example:
192.168.29.47 Computer_A.thermocalc.se.
 8. Save the changes.
 9. In the host file, there is an example of how the operating system (Windows or Linux) wants the line in the hosts file to look like.

macOS Installations: Running the License Initialization Script

As part of the Standalone installation of Thermo-Calc, the Setup runs a license initialization script. If this part of the installation process did not complete properly for a standalone installation, you must manually run the license initialization script. You need the administrator username and password for these steps.

HOW TO RUN THE SCRIPT

For this script to successfully initialize the license, the license file must be called **lservrc** and be located in the folder:

`/Users/Shared/Thermo-Calc`

► ["Default Directory Installation Locations" on page 15](#)

1. Open a terminal window. The **Terminal** application is in the `/Applications/Utilities` folder.
2. At the prompt, enter this command:

```
$ sudo /Applications/Thermo-Calc-  
2020a.app/Contents/Resources/license-initialization-macOS-  
x86_64.sh
```

For demo installations, the path should be `/Applications/Thermo-Calc-2020a-Demo.app/Contents/Resources/ license-initialization-macOS-x86_64.sh`.

If you are not already logged in as an administrator, you probably cannot run the `sudo` command. If this is the case, then you can use the `su` command in the terminal window to login as an administrator. Contact your local system administrator for help.

3. Enter the administrator password and press `Enter`.
4. When you restart your computer and run the license initialization script, you are ready to start using Thermo-Calc.



If you did not install a license file during this procedure, you can still start Thermo-Calc although you will get the **No license file found** message.

Linux Installations: Running the License Initialization Script

As part of a Standalone installation of Thermo-Calc, the Setup runs a license initialization script. If you get a warning message during the standalone installation Unable to run post-installation script, run the license initialization script as root after the installation, then you need to manually run the script as root.

OPENSUSE ADMINISTRATION (SUDO) USERS

Note the following if you are a sudo user (administrator) in openSUSE installing Thermo-Calc using this command:

```
sudo ./linux-installation-x64-6.0.0.17347.run
```

When this command is used, you will do a text-based installation instead of having a graphical interface to guide you. The information is the same, just without the user interface.

HOW TO RUN THE SCRIPT



For this script to successfully initialize the license, the license file must be called **lservrc** and be located in the directory where you have installed Thermo-Calc.



["Default Directory Installation Locations" on page 15](#)

1. In the console, go to the Thermo-Calc installation directory.

- The license file is put in `/home/<user>/Thermo-Calc` if you are installing as a non-root user, where `<user>` is your user name.
- If you are installing as root, then this directory is `opt/Thermo-Calc/`.

2. Enter this command:

```
$ sudo sh license-initialization-linux.sh
```

If you are not able to execute the `sudo` command because you are not on the sudoers list, you must log in as a root user with the command `su`, and then use `sh` to run the license initialization script. For example, on a 64-bit computer, enter the following:

```
$ sh license-initialization-linux.sh
```

3. Log out of Thermo-Calc and then log back in to save these changes.

Uninstalling Thermo-Calc

In this section:

| | |
|-----------------------------------------------------|----|
| Uninstalling Thermo-Calc | 65 |
| Uninstalling Standalone Versions of TC-PRISMA | 66 |

Uninstalling Thermo-Calc

WINDOWS 10

1. From the **Control Panel** Desktop app, go to **Programs → Programs and Features → Uninstall or change a program**.
2. In the list of programs, locate the version of Thermo-Calc you want to uninstall. Click to highlight that row.
3. Click **Uninstall/Change**.
4. In the **Setup** window, **Uninstallation Mode** dialog box, choose to uninstall the **Entire application** or **Individual components**. Follow the instructions to finish.

MAC

Deleting the program from the Applications folder does not remove the program from your operating system. Run the **Thermo-Calc-*<version>*-uninstaller** program located in the Applications folder. This is also applicable to the Demo version of the software.

1. Go to the **Applications** folder and double click the file that starts with **Thermo-Calc-*<version>*-uninstaller**. Enter the administrator's user name and password.
2. Click **Yes** to choose **Entire application** or select individual components. Otherwise click **No** to quit.
3. The **Uninstalling Thermo-Calc** window shows the progress. Click **OK** when prompted.

LINUX

1. To start the uninstallation procedure, in the Thermo-Calc installation directory use the command

```
./Thermo-Calc-2020a-uninstaller.run
```

For *Thin Client* installations, use the command

```
./Thermo-Calc-client-2020a-uninstaller.run
```

2. To remove the whole application, including all its components, select **Entire application** and click **Forward**, or to remove specific components, select **Individual components** and click **Forward**.



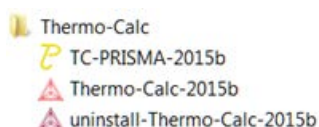
If you intend to reinstall Thermo-Calc 2020a it is important to remove the environmental variable TC20A_HOME by logging out and back into the Linux user account.

Uninstalling Standalone Versions of TC-PRISMA

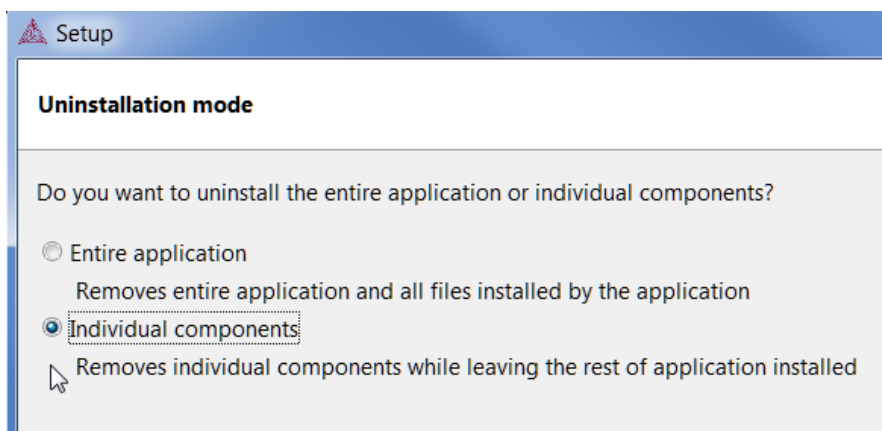


As of Thermo-Calc version 2016a, TC-PRISMA is no longer a standalone program. It is integrated into the Thermo-Calc Graphical Mode and considered an add-on module called the Precipitation Module. It is also available for all platforms (Windows, Mac and Linux). If you have older versions of the TC-PRISMA software that you want to uninstall, follow these instructions.

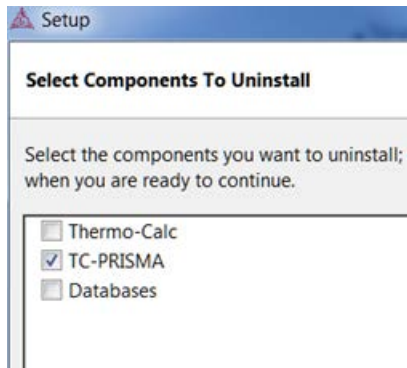
1. Go to the Thermo-Calc uninstaller. For example, in Windows 7, go to **Start → All Programs → Thermo-Calc** or in Windows 10 go to **Start → All Apps → Thermo-Calc**.
2. Click **uninstall-Thermo-Calc-2015b** (or the version of TC-PRISMA you have).



3. In the **Setup** window, click **Individual components**. Click **Next**.



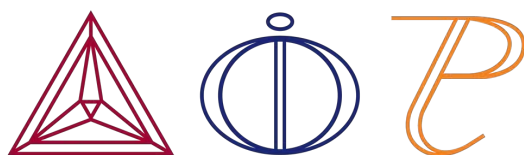
4. Select the **TC-PRISMA** check box.



5. Click **Next** and then **OK** when the software component is uninstalled.

The Thermo-Calc Software

Thermo-Calc Version 2020a



About the Thermo-Calc Software

In this section:

| | |
|---------------------------------------------------------|----|
| The Thermo-Calc Software | 3 |
| About the Thermo-Calc Add-on Modules | 3 |
| Graphical Mode vs Console Mode | 5 |
| Graphical Mode Activities vs Console Mode Modules | 7 |
| Graphical Mode vs Console Mode: Calculation Types | 9 |
| About the File Types and Formats | 12 |
| Displaying Thermo-Calc License Information | 13 |

The Thermo-Calc Software

The Thermo-Calc software is a sophisticated database and programming interface package used to perform thermodynamic calculations. It can calculate complex homogeneous and heterogeneous phase equilibria, and then plot the results as property diagrams and phase diagrams.

The Thermo-Calc software (also referred to as the *Thermo-Calc program* or *the software* to distinguish it from the company name) fully supports stoichiometric and non-ideal solution models and databases. These models and databases can be used to make calculations on a large variety of materials such as steels, alloys, slags, salts, ceramics, solders, polymers, subcritical aqueous solutions, supercritical electrolyte solutions, non-ideal gases and hydrothermal fluids or organic substances. The calculations take into account a wide range of temperature, pressure and compositions conditions.

About the Thermo-Calc Add-on Modules

The Thermo-Calc program also includes add-on modules as briefly described below and at the links to our website.

- The Diffusion Module (DICTRA) is used to simulate diffusion controlled transformations in multicomponent systems. You can find more about it [on our website](#).
- The Precipitation Module (TC-PRISMA) is used to simulate diffusion controlled multi-particle precipitation process in multicomponent and multi-phase alloy systems. You can find more about it [on our website](#).
- The Process Metallurgy Module is used to set up calculations used in steel making and other metallurgical industries. You can find more about it [on our website](#).

Diffusion Module (DICTRA)

The Diffusion Module (DICTRA) is an add-on module to Thermo-Calc. It is used for simulation of diffusion controlled transformations in multicomponent systems. The simulation calculations are both time- and space-dependent. The Diffusion Module (DICTRA) is available in both Graphical Mode (as the *Diffusion Calculator*) and Console Mode (as the *DICTRA module*).

The Diffusion Module (DICTRA), which is often just referred to as DICTRA, is ideally suited to solve diffusion simulations that include a moving boundary (*Stefan problems*). The multicomponent diffusion equations in the various regions of a material are solved under the assumption that thermodynamic equilibrium holds locally at all phase interfaces. Simulations are one-dimensional and three different geometries can be performed: planar, cylindrical, and spherical.

Examples of cases that have been simulated using the Diffusion Module (DICTRA) include:

- Microsegregation during solidification
- Homogenization of alloys
- Growth/dissolution of carbides, nitrides and intermetallic phases
- Coarsening of precipitate phases
- Interdiffusion in compounds, e.g. coating systems
- Austenite to ferrite transformations in steel
- Carburization, nitriding and carbonitriding of high-temperature alloys and steels
- Post weld heat treatment
- Sintering of cemented-carbides

Precipitation Module (TC-PRISMA)

The Precipitation Module, or TC-PRISMA, is an add-on module to Thermo-Calc and it is available in Graphical Mode as the *Precipitation Calculator*.

The module treats concurrent nucleation, growth/dissolution and coarsening under arbitrary heat treatment conditions in multi-component and multi-phase systems using Langer-Schwartz theory and the Kampmann-Wagner numerical approach. It is a general computational tool for simulating kinetics of diffusion controlled multi-particle precipitation processes in multicomponent and multiphase alloy systems.

You can use the Precipitation Module for:

- Concurrent nucleation, growth/dissolution and coarsening of precipitates
- Temporal evolution of particle size distribution
- Average particle radius and number density
- Volume fraction and composition of precipitate
- Nucleation rate and coarsening rate
- Time-Temperature-Precipitation (TTP) diagrams
- Continuous-Cooling-Transformation (CCT) diagrams
- Estimation of multi-component interfacial energy

Process Metallurgy Module

The Process Metallurgy Module is an add-on module to Thermo-Calc and it is available in Graphical Mode as the *Process Metallurgy Calculator*. The module is designed to model reactions that occur in metallurgical processes. It is based on the global equilibrium of the process. Although primarily used in steelmaking and steel refining processes (such as basic oxygen furnaces, electric arc furnaces, ladle furnace metallurgy and so forth), applications are not limited to steelmaking. The main difference compared to the a standard Equilibrium Calculator is that it is easy to handle the different materials present in a metallurgical process. The is especially true for the slag composition that is based on components.

Both isothermal and adiabatic calculations are possible. Adiabatic calculations assume no heat and mass exchange with the environment during the equilibrium reaction.

You can use the Process Metallurgy Module to calculate:

- The equilibrium between predefined steels and slags
- Desulfurization, dephosphorization, decarburization
- Any partition coefficient
- Slag characteristics, such as slag basicity or sulphur capacity
- The fraction of liquid and solid in the slag
- The temperature change in an adiabatic process

The module requires both a valid Maintenance and Support Subscription (M&SS) and a license for the TCS Metal Oxide Solutions Database (TCOX).

Graphical Mode vs Console Mode

There are two interfaces available in Thermo-Calc: *Graphical Mode* with a graphical user interface (GUI) and *Console Mode*, which uses a command line interface. Thermo-Calc and the Diffusion Module (DICTRA) are available in both modes, and the Precipitation Module (TC-PRISMA) is only available in Graphical Mode.

If you are a new user, Graphical Mode is a good way to learn how to work with Thermo-Calc. Depending on what you want to simulate, Console Mode can have more functionality but until you are comfortable with the concepts, it is recommended you start in Graphical Mode.



In Graphical Mode calculations are set up, carried out, and visualized as part of a *project*. The steps in the project are performed with *activities*. There are templates and a Wizard available to guide you through the process of defining the project.

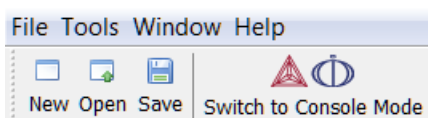


In Console Mode you work with *modules*, which are managed using commands typed at a prompt. Some modules, called *response-driven modules*, ask you a series of questions that typically take you through the process of defining your system, setting calculation conditions, performing calculations and plotting the results.

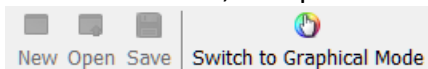
SWITCHING BETWEEN MODES

The first time you open Thermo-Calc, it defaults to Graphical Mode. For any future instance it defaults to the last mode used.

Along the top of the GUI is the **GRAPHICAL MODE TOOLBAR** where you switch between modes.



In Console Mode, except for the **SWITCH TO GRAPHICAL MODE** button, the toolbar is not used.



See ["Menu, Toolbar and Keyboard Shortcuts" on page 4](#) for information about the **Tools**, **Window** and **Help** menus, which are available in both modes.

FILE EXTENSIONS

The file extensions are different based on the mode you are in (Graphical vs. Console). In Console Mode the extensions are also based on whether you are working with Thermo-Calc or the Diffusion Module (DICTRA).



In Graphical Mode, the Thermo-Calc project files have the extension *.t_{cu}. This includes the examples for the add-on Diffusion Module (DICTRA) and Precipitation Module (TC-PRISMA).



In Console Mode, Thermo-Calc macro files have a *.TCM extension and the Diffusion Module (DICTRA) file extension is *.DCM. In addition to macro files in Console Mode there are also *Log* files and *Workspace* files, which also differ.

CAN I WORK WITH BOTH MODES AT THE SAME TIME?

The two modes can be run simultaneously, but there is no communication between them.

What you do in Graphical Mode does not affect the state of the Console Mode session and vice versa. One exception is the plot settings. See ["Global Settings: Graphical and Console Mode Plotting" on page 47](#).

DATA OPTIMIZATION AND THERMODYNAMIC / KINETIC ASSESSMENTS



Although many calculations can be done in either mode, data optimization and thermodynamic or kinetic assessments are only available in Console Mode.

Graphical Mode Activities vs Console Mode Modules

- ▶ Graphical Mode: ["About the Activity Nodes" on page 9](#)
- ▶ ["Console Mode Modules" on page 9](#)

Although many calculations can be done in either Graphical Mode or Console Mode, only data optimization and thermodynamic or kinetic assessments are available in Console Mode. Conversely, only the Property Model, Precipitation and Process Metallurgy Calculators are available in Graphical Mode.

Below is a brief description of the available modules. The specific modules, using the names in the table, are accessed through Console Mode. For Graphical Mode, the underlying principles, and the final calculations, are incorporated into the projects and activity nodes. Some modules require additional licenses.

GRAPHICAL MODE ACTIVITIES VERSUS CONSOLE MODE MODULES

| GM Activity | CM Module (Short Name) | Primary Functions |
|----------------------|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Binary Calculator | BIN | Calculate binary phase diagrams. Access to specific databases designed for BIN, such as TCBIN, is required. |
| System Definer | DATA | Select appropriate databases, define chemical systems and retrieve the data required for calculations. |
| Diffusion Calculator | DICTRA | Run simulations of diffusion controlled transformations in Thermo-Calc using the Diffusion Module (DICTRA). An additional license is required for this feature. |
| — | DIC_PARROT | This is the data optimization module for the Diffusion Module (DICTRA). It allows you to assess experimental data and use such data to optimize calculations. An additional license is required for this feature. |

| GM Activity | CM Module (Short Name) | Primary Functions |
|--------------------------------|------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| – | ED_EXP | Part of the PARROT submodule, use it to edit experimental data points to make reliable optimizations. |
| This is the calculation engine | GIBBS or GES | Handles thermodynamic models and quantities. Generally you do not need to use this module, but you can get information about models, and list, add or amend the thermodynamic parameters in use. |
| – | PARROT | A data optimization module to assess experimental data and use the data to optimize calculations. |
| Precipitation Calculator | – | Set the conditions for, and perform, a precipitation calculation. |
| Property Model Calculator | – | Predict and optimize material properties based on their chemical composition and temperature. There are preconfigured General Models and Steel Models available. |
| Equilibrium Calculator | POLY | Equilibrium calculation module. Specify conditions and make calculations. |
| Plot Renderer | POST | This is a submodule to POLY and is for post-processing and plotting of calculation results. Modify property and phase diagrams, add labels, change the diagram colors and so forth. |
| Ternary Calculator | POTENTIAL | Calculate and plot gas potential diagrams in a ternary system. The potential of two gas species are used as the diagram axes. |
| – | POURBAIX | Calculate and plot pH-Eh diagrams (Pourbaix diagrams) and property diagrams for heterogeneous interaction systems involving aqueous solutions. |
| Process Metallurgy Calculator | – | Use this to set up calculations for steel and slag. Define the composition of a steel and slag system using material groups: one each for steel (or another user-defined metal), slag and gas. |
| – | REACTOR | Simulate chemical reaction processes in several feed-forward steady-state stages or in several dynamic stages. |
| Scheil Calculator | SCHEIL | Simulate and plot Scheil-Gulliver solidification processes with no diffusion in the solid phases and with/without consideration of back diffusion of interstitial components (such as C, N, O, S). |
| – | SYS | In Console Mode, interact with the operating system and change environmental settings. Create and execute macro files. |
| – | TAB | Tabulate properties of chemical reactions and substances (stoichiometric or solution phases). |
| Ternary Calculator | TERN | Calculate ternary phase diagrams. |

Graphical Mode vs Console Mode: Calculation Types

▶ ["The Calculation Types in Graphical Mode" on page 23](#)

▶ ["Calculations" on page 35](#)

When you are using Thermo-Calc and the add-on modules, you generally first set up a system, select the databases to use, and then define various parameters related to the simulation you want to conduct. Once this is set up you decide what calculation type to perform, choose a plot type (or a table for single equilibrium, for example) to use and then eventually get a result.

How Thermo-Calc handles the calculation behind the scenes is the same whether you use Graphical Mode or Console Mode. However, there are differences with the workflow and for historical reasons some calculation types are named differently based on whether you are in one mode or another. In addition, the plot types (diagrams) you choose to output the information are also different based on whether you are in Graphical or Console Mode. These plot types are often based on the type of calculation being done, where in some cases you can only do it in one mode and not the other. For example, precipitation calculations are only available with the Precipitation Calculator, which is only available in Graphical Mode, but you can do diffusion calculations in both Graphical and Console Mode.

COMPARISON OF CALCULATION TYPES IN GRAPHICAL MODE VS CONSOLE MODE

The table lists most of the calculation types that you will want to perform based on whether it is in Graphical Mode or Console Mode. The first column is primarily based on the calculation types you can select when working in Graphical Mode and when using the various calculators as indicated in the second column. The third column is the module or command in Console Mode that you would use to perform the same, or similar, type of calculation.

| Calculation Type | Graphical | Console | Definition |
|--------------------------|------------------------|--------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Equilibrium calculations | Equilibrium Calculator | POLY3 module | An equilibrium defines the amount(s) and composition(s) of one or several phases that have the minimum Gibbs energy at a given temperature and pressure. A prerequisite for a successful equilibrium calculation is that the number of degrees of freedom according to Gibb's phase rule must be zero. This means that the right number of independent conditions must be set in order to successfully be able to calculate an |

| Calculation Type | Graphical | Console | Definition |
|---------------------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | | | equilibrium. |
| Single equilibrium | Property Model Calculator (Equilibrium model) and Equilibrium Calculator | POLY3 module | <p>To calculate a single equilibrium. The results from this calculation are displayed as follows:</p> <ul style="list-style-type: none"> Graphical Mode: In the Results window for a Table Renderer or in the Event Log window (for the Property Model Calculator) Console Mode: With the LIST_EQUILIBRIUM command. |
| Single (no axes) | Property Model Calculator and Process Metallurgy Calculator | POLY3 module | <p>To calculate a single point. The results from this calculation are displayed as follows:</p> <ul style="list-style-type: none"> Graphical Mode: In the Results window for a Table Renderer or in the Event Log window. Console Mode: With the LIST_EQUILIBRIUM command. |
| One axis | Property Model Calculator, Equilibrium Calculator and Process Metallurgy Calculator | POLY3 module | To vary a quantity on the X-axis. |
| Property diagrams | One axis: available with Equilibrium Calculator or Property Model Calculator | POLY3 module, STEP command | A property diagram is calculated by stepping one of the conditions that were defined for the equilibrium calculation and plotting some other property against this variable. For example stepping through temperature and plotting equilibrium composition of a certain phase, or stepping through composition and plotting equilibrium phase fractions, and so forth. |
| Phase diagrams | Equilibrium Calculator, Binary Calculator, and Ternary Calculator | POLY3 module, MAP command, BINARY module, and TERNARY module | A phase diagram is mapped within a specific space constructed by two (or more) independent mapping variables. These are mostly temperature and composition, but can be many other, such as temperature and pressure, activity of oxygen and activity of sulphur, and so forth. |
| Scheil calculations | Scheil Calculator | Scheil module | Simulate a non-equilibrium transformation or partial-equilibrium transformation, also called a Scheil-Gulliver solidification. |

| Calculation Type | Graphical | Console | Definition |
|----------------------------|--------------------------------------------------------------------------------------|-------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Gibbs energy curves | Binary Calculator | BINARY module | To calculate at a constant temperature over the whole composition range. |
| Activity curves | Binary Calculator | BINARY module | To calculate at a constant temperature over the whole composition range. |
| Phase fractions | Binary Calculator | BINARY module | To calculate as a function of temperature at a constant composition. |
| Isothermal section | Ternary Calculator | TERNARY module | To calculate the ternary system for the whole composition range at a constant temperature. |
| Monovariant lines | Ternary Calculator | TERNARY module | To calculate the variation of the liquid compositions with temperature. |
| Liquidus projection | Ternary Calculator | TERNARY module | The projection liquid surface and the monovariant lines are calculated over the given temperature range. |
| Potential diagrams | not available | Potential Diagram module and POLY3 module | A potential diagram uses the activities of two major species in the gaseous mixture phase as mapping variables. For example, use this for a metal-oxide/sulphide-gas interaction system to calculate a diagram based on a specific temperature and pressure . |
| T0 temperature simulations | not available | POLY3 module | The T0-temperature is the temperature at which two phases have the same Gibbs energy for a certain composition for a certain alloy composition. |
| Paraequilibrium | not available | POLY3 module | A paraequilibrium is a partial equilibrium where one interstitial component, such as carbon (C) and nitrogen (N), in a multicomponent alloy can diffuse much faster than the other components (the substitutional elements, including the matrix element and alloying elements). |
| Grid | Property Model Calculator, Equilibrium Calculator, and Process Metallurgy Calculator | not available | With the Equilibrium Calculator, it computes the equilibrium of each grid point in a two-dimensional grid. With the Property Model Calculator, it evaluates two axis variables of the selected quantities in the specified range and number of steps. |
| Min/Max | Property Model Calculator | not available | Evaluates the property model(s) for all variations of the selected quantities at the |

| Calculation Type | Graphical | Console | Definition |
|-------------------------------------|-------------------------------------------------------------|--------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | | | given limits. |
| Uncertainty | Property Model Calculator and Process Metallurgy Calculator | not available | Evaluates the property model(s) where the values of the quantities are sampled from Gaussian distributions. |
| Aqueous solutions, Pourbaix diagram | Equilibrium Calculator | Pourbaix Diagram module, POLY module | A Pourbaix diagram is a kind of phase diagram that shows the stability boundaries for a metal-aqueous interaction system. The phase boundaries are shown as a function of pH (acidity) and Eh (standard hydrogen electronic potential). |
| Tabulation reaction | not available | TAB module | To tabulate thermodynamic functions of any type of substance, stoichiometric phase or solution phase, or reaction. |
| Diffusion simulation | Diffusion Calculator | DICTRA monitor | Detailed simulation of diffusion controlled reactions in multi-component systems. |
| Isothermal | See below | POLY3, DICTRA monitor | Isothermal calculations in general can be done in all Console Mode modules, for example an Isothermal diffusion in DICTRA monitor and an isothermal calculation in POLY3 using the STEP command. |
| Isothermal and non-isothermal | Precipitation Calculator | See above | You can calculate nucleation, growth/dissolution and coarsening of particles size classes under these conditions: isothermic (precipitation simulation at constant temperature) or non-isothermic (precipitation simulation with user-defined temperature profile). |
| TTT and CCT | Precipitation Calculator | not available | The TTT (Time-Temperature-Transformation) and CCT (Continuous Cooling Transformation) diagram can be simulated for one or more particles. |

About the File Types and Formats

The file formats (and the file extensions / suffixes) are based on whether you are working in Graphical or Console Mode, and in Console Mode, whether you are working with Thermo-Calc and/or the Diffusion Module (DICTRA).

GRAPHICAL MODE

In Graphical Mode you work with one file type, a *project* file, which has a *.tcu file extension. This is applicable to Thermo-Calc and the add-on Diffusion and Precipitation modules.

CONSOLE MODE

In Thermo-Calc Console Mode there are file *types*—**macro** (including log files) and **workspace**—and *extensions* —*.TCM, *.POLY3, *.GES5, *.PAR, *.POP, and *.EXP.



A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.



Workspace files are not currently available with GES6.



["Working with the Console Mode File Types" on page 20](#)

Displaying Thermo-Calc License Information

You can start (and install) the software without a valid Thermo-Calc license but you cannot do any calculations. To show information about the available and installed licenses, from the main menu select **Help → Show License Info**.

This is an example of part of a License Information window for a network installation. It only shows the fields you would expect to see as the details are unique for each installation.

License Information

License diagnostics program
build: 19853 created: Mon Apr 08 14:24:19 2019

Log generated at: 24-04-2019 10:59:13

Safenet environment variables

LSHOST:

LSERVC:

Local (client) info

hostname:

license version:

ethernet: #1

ethernet: #2

ip address: #1

ip address: #2

dns name: #1

dns name: #2

short locking code:

short lock name:

short lock IP-address:

short lock ethernet:

NETWORK LICENSES

For a *network* license, under each license type with instances checked out, there is a list of who checked out each license.



In Graphical Mode, an instance is checked out when an Equilibrium Calculator activity is created, and checked back in when that Equilibrium Calculator is removed. For the add-on Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA) this also applies to the Diffusion Calculator and the Precipitation Calculator.



In Console Mode, an instance is checked out when you enter the POLY module and is checked back in when you exit the POLY module.

- The **Features** column is a list of the specific software, databases and API licenses purchases.
- The **Version** is an internal version number for the feature.

-
- The **number of licenses** column is how many instances of each license type available to be checked out simultaneously.
 - The **in use** column shows how many license instances are checked out.

CONSOLE MODE LICENSE RESTRICTIONS

- If you start Thermo-Calc without a valid Thermo-Calc license you cannot leave the SYS module.
- If all the licenses are checked out for a network client installation of Thermo-Calc, you may not be able to enter the POLY or DICTRA modules until a license is available.
- To enter the DICTRA and the DIC_PARROT modules, you need a valid Diffusion Module (DICTRA) license key.
- If you enter and use either the DIC_PARROT module or the PARROT module, then you cannot enter the other module in the same session. You must close down Thermo-Calc and launch the program again to enter the other data optimization module.

NETWORK COMPUTER LICENSE RESTRICTION

If you have a network computer installation of Thermo-Calc, then you may not be able to do any calculations even if you have access to a valid network license file. This is because others who are part of your network installation may have checked out all allowed instances of the software.

If you are running a network installation of Thermo-Calc, you can see how many instances of the client licenses are currently checked out and how many of them are left. You can also see which client computers have checked out the licenses.

About the Documentation and Examples

In this section:

| | |
|-----------------------------------------------|----|
| Examples, Manuals and Materials Folders | 17 |
| About the PDF Documentation Folder | 20 |
| About the Examples | 23 |
| Help Resources | 25 |
| Typographical Conventions | 27 |

Examples, Manuals and Materials Folders

There are several ways to access the examples, manuals (containing PDF documentation) and materials data folders.

| | Main Menu | System Definer | From the Windows Start Menu | On your computer | Website |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|----------------|-----------------------------|------------------|---------|
| Manuals (PDF documentation, DATAPLOT EXP files, and Property Model Framework Tutorial Examples) | x | - | x | x | x |
| SDK (TCAPI, TC-Python and TQ-Interface APIs)* | x | - | - | x | x |
| Examples (project and macro files) | x | - | x | x | x |
| Materials | - | x | x | x | x |
| Property Models | - | - | - | x | - |
| Process Metallurgy Materials** | - | - | - | x | - |
| <p>* The SDK folder is installed when you have selected this custom option during installation and have a license for the applicable SDK.</p> <p>** The Process Metallurgy Module user-defined material compositions are saved from the Process Metallurgy Calculator and managed from the Tools → Options menu.</p> | | | | | |

FROM THE MAIN MENU

Once your Thermo-Calc software is installed you can open the Examples and PDF documentation (Manuals) from the main menu:

- To open the Manuals folder select **Help → Manuals Folder**. Note for Linux openSUSE users: This link is not functional. To access the folder, navigate to the default location based on your installation type
- To open the Examples based on whether you are in Console Mode or Graphical Mode, select **File → Examples Files** or **Help → Examples Files**.

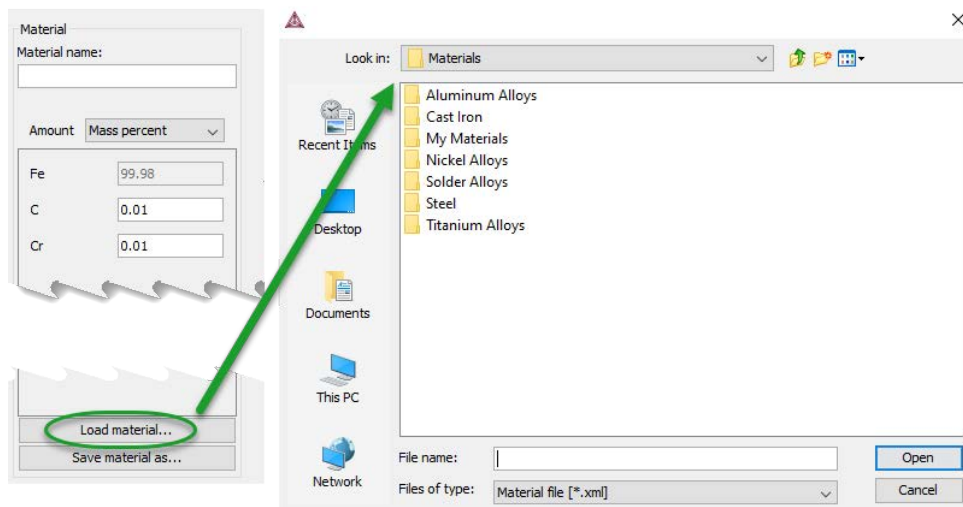
FROM THE SYSTEM DEFINER (MATERIALS ONLY)

When you are working with the System Definer you can open the default **Materials** folder included with your installation.

At the bottom of the window under **Material**, click **Load material** to navigate to a material file.



There is a separate folder for materials saved using the Process Metallurgy Calculator. See [Process Metallurgy Materials](#).



The default directory where these files are stored is based on operating system:

| Operating system | Materials installation directory |
|------------------|----------------------------------------------------------------------------------------------------------------------------------------------------|
| Windows | C:\Users\<user>\Documents\Thermo-Calc\2020a\Materials |
| Linux | On Linux all user files are installed where the program is installed. If installed as root the default is: /opt/Thermo-Calc/2020a/Materials |
| Mac | /Users/Shared/Thermo-Calc/2020a/Materials |

START MENU (WINDOWS ONLY)

On Windows, once Thermo-Calc is installed, you can locate the Examples and Materials folders, plus all the Manuals using the shortcuts located in the Start menu. Go to **Start → All**

Programs or **All Apps** → **Thermo-Calc** and click **Examples, Manuals, or Materials** as required to open the applicable folder.

ON YOUR COMPUTER (ALL OPERATING SYSTEMS)

The PDFs, example files and materials xml files are included with your installation in a folder location based on the operating system.

In the table, *<user>* stands for the username and *<version>* for the version of Thermo-Calc, for example 2020a.

Windows File Paths

| User type | Default directory |
|---------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Administrator | Software Program Files\Thermo-Calc\<version> Examples, Manuals, Materials, Property Models, Process Metallurgy Materials and SDK folders: Users\Documents\Thermo- Calc\<version> |

Mac File Paths

| User type | Default directory |
|-------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Administrator (user name and password required) | Examples, Manuals, Materials, Property Models, Process Metallurgy Materials and SDK folders: /Users/Shared/Thermo-Calc/<version> To go to this folder, in Finder, from the Go main menu select Go to folder . Enter the above file path and click Go . |

Linux File Paths

| User type | Default directory |
|---------------|-----------------------------------|
| Non root user | home/<user>/Thermo-Calc/<version> |
| Root user | usr/local/Thermo-Calc/<version> |

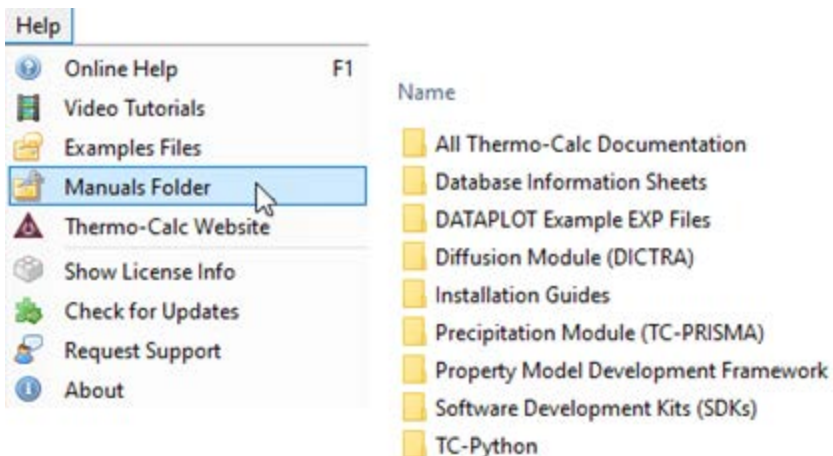
WEBSITE

You can download the PDF documentation and examples from the website.

1. Go to <https://www.thermocalc.com/>.
2. From the menu, select **Support** → **Documentation** and navigate to the applicable section.

About the PDF Documentation Folder

There is PDF documentation available as part of your installation. This is the same information as that contained in the online help, just in a different format. The contents of each folder are described below.



All Thermo-Calc Documentation

The *Thermo-Calc Documentation Set* is one large PDF that includes the information needed to work with the Thermo-Calc software. By having all content in one PDF it enables you to search the content just like you would when in the online help, although this PDF does not include all the add-on module and SDK content.

The documentation set includes:

- Thermo-Calc installation guides including Windows, Mac and TC-Python Quick Install Guides
- User guides for both Graphical Mode and Console Mode
- *Data Optimization User Guide* - Console Mode only
- *Database Manager User Guide* - Console Mode only
- *DATAPLOT User Guide* - Console Mode only
- *Pourbaix Diagrams Educational Material*
- *Thermo-Calc Console Mode Example Macros*
- *Property Model Development Framework Guide* - Graphical Mode only

Database Information Sheets

The text contained in the extended information database information sheets is included in the online help system. PDF copies are located in this sub-folder. You can also download these from the Thermo-Calc [website](#).

DATAPLOT Example EXP Files

The examples are available as supplementary information as described in the *DATAPLOT User Guide*, which you can find in either the online help, Thermo-Calc Documentation Set or Diffusion Module (DICTRA) Documentation Set.

Diffusion Module (DICTRA)

The Diffusion Module Documentation Set is one large PDF that contains information you need to work with this add-on module. By having all content in one PDF it enables you to search the content just like you would when in the online help, although this PDF does not include any installation or SDK content.

The documentation set includes:

- All the user guides available in the Thermo-Calc Documentation Set
- Diffusion Module (DICTRA) user guides and quick start guides for both Graphical Mode and Console Mode

The following guides are also available separately in this folder as well included in the documentation set:

- *Diffusion Module Quick Guide - Console Mode*
- *Diffusion Module Quick Guide - Graphical Mode*
- *Diffusion Module (DICTRA) Console Mode Example Macros*

Installation Guides

Includes the quick install guides for Standalone Windows and Mac installations as well as the full installation guide for all platforms and installation types. A quick install guide for TC-Python is also there.

Precipitation Module (TC-PRISMA)

There is a stand-alone user guide in this folder. Use the Thermo-Calc Documentation Set for all other details you need to work with this add-on module, which treats concurrent nucleation, growth/dissolution and coarsening under arbitrary heat treatment conditions in multicomponent and multi-phase systems using Langer-Schwartz theory and the Kampmann-Wagner numerical approach.

Property Model Development Framework

The PDF guide contains details about setting up a development environment so you can build custom property models in Thermo-Calc.

The folder also includes two tutorial Python files you can copy and use in your own custom property models. The examples are available as supplementary information as described in the *Property Model Development Framework Guide*.

Software Development Kits (SDKs)



The TC-Python API HTML documentation is stored in its own folder. It is also available from our [website](#). In this folder you will find the PDF version of the help.

- **TQ-Interface Programmer Guide:** The TQ-Interface is available as a way to make Thermo-Calc an integral part of application programs such as those for process

simulation, microstructure evolution modeling and materials property prediction.

- **TC Toolbox for MATLAB® Programmer Guide:** Use this to enable communication between Thermo-Calc and MATLAB® to be able to retrieve thermodynamic and kinetic quantities.
- **TC-API Programmer Guide:** This is the Thermo-Calc API that can be used by programmers to set up your own applications to work with Thermo-Calc.

TC-Python (SDK)

TC-Python is an SDK and you can search and use the special HTML file located in this folder. Double-click the Index.html file to open it. This help is also available via our [website](#).

About the Examples

To learn more about how to use the software you can open and run the example projects (Graphical Mode) and macro files (Console Mode).

GRAPHICAL MODE EXAMPLES

Graphical Mode examples are available for Thermo-Calc and the add-on Diffusion Module (DICTRA), Precipitation Module (TC-PRISMA), and Process Metallurgy Module. These are in the format of project files (*.tcu).

CONSOLE MODE EXAMPLES

Console Mode examples are available for Thermo-Calc and the Diffusion Module (DICTRA). The *macro* files are in the format of *.TCM and *.DCM, respectively.



There are other file types when you are working in Console Mode. See ["Working with the Console Mode File Types" on page 20](#) and *About the File Formats* in the *Diffusion Module Quick Start Guide*.

Examples by Product

Thermo-Calc Examples

A description of the Thermo-Calc examples, and how to access them, is based on whether

you are using Graphical Mode or Console Mode.

 ["Graphical Mode Examples" on page 239](#)


 ["Thermo-Calc Console Mode Examples " on page 414](#)

Diffusion Module (DICTRA) Examples

A description of Diffusion Module (DICTRA) examples, which are available for both Graphical Mode and Console Mode, is included in both the Thermo-Calc and Diffusion Module (DICTRA) documentation.

 For Graphical Mode, see ["Diffusion Module \(DICTRA\) Graphical Mode Examples" on page 308](#)

► For Console Mode, search the help or go to the Diffusion Module (DICTRA) documentation set.

 All the macro files and the outputs are also combined into one file that you can search and read. This is included with your installation as a PDF (go to **Help > Manuals folder > Diffusion Module (DICTRA)** and open *Diffusion Module Console Mode Example Macros*).

Precipitation Module (TC-PRISMA)

A description of examples using the Precipitation Calculator, which is only available in Graphical Mode, is included in both the Thermo-Calc and Precipitation Module (TC-PRISMA) documentation.

 ["Precipitation Module \(TC-PRISMA\) Graphical Mode Examples" on page 330](#)

Process Metallurgy Module Examples

A description of examples using the Process Metallurgy Calculator, which is only available in Graphical Mode, is included in the Thermo-Calc documentation.

 ["Process Metallurgy Examples Collection" on page 288](#)

TC-Python Examples

A brief description of the TC-Python SDK examples, and how to access these, is available in the Help.

TQ-Interface and TC-Toolbox for MATLAB Examples

There are examples for the TQ-Interface and TC-Toolbox for MATLAB available as described in "[Examples, Manuals and Materials Folders](#)" on [page 17](#). You can also find information about these in the respective user guides or by searching the online help.

Watch the Video Tutorials



Many of the Graphical Mode examples have video tutorials available both on [our website](#) and our [YouTube channel](#).



You can access video tutorials in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or you can go to the [website](#) or our [YouTube channel](#).

Help Resources

'Online' Help: No Internet Required


To access online help in a browser, open Thermo-Calc and press <F1> on the keyboard, or select **Help → Online Help**.

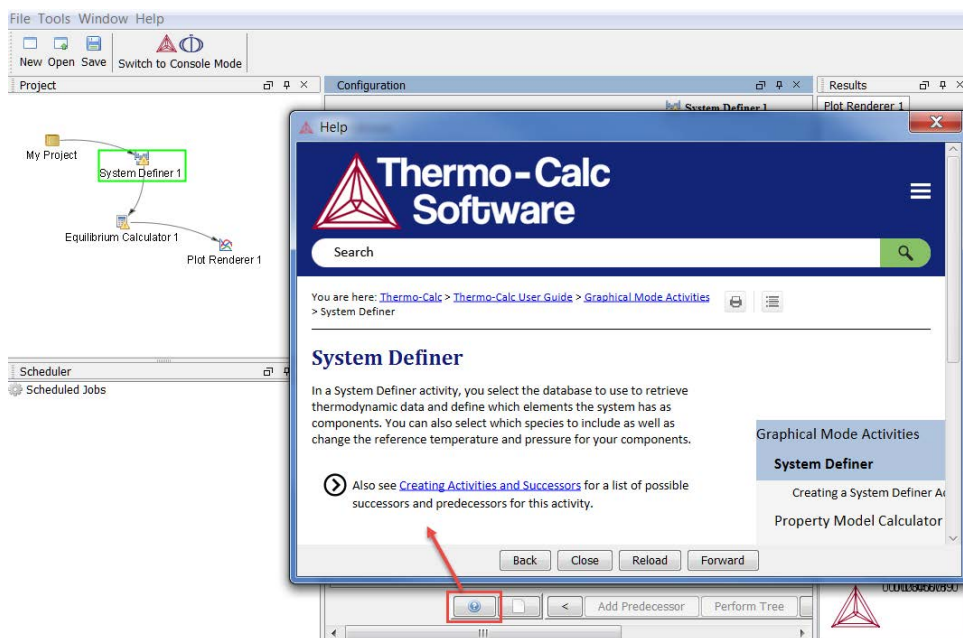
The content opens in a browser but uses local content so you don't need an Internet connection except for links to external websites.

Context Help (Graphical Mode Only)

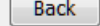





When you are in Graphical Mode, you can access feature help (also called *topic-sensitive* or *context help*) for the activity nodes in the tree.

1. In the **Project** window, click a node. For example, **System Definer**.
2. In the lower left corner of the **Configuration** window, click the help button .
3. The **Help** window opens to the relevant topic.



The window that opens has the same content as the help you access in the browser. There are these extra navigation buttons in this view.

- Use the buttons on the bottom of the window,    , to navigate **Back** and **Forward** (these are only active once you have started using the help to load pages and create a history), to **Close** the window, and **Reload** the original content.

Console Mode Help



Console Mode is for Thermo-Calc and the Diffusion Module (DICTRA).

In Console Mode at the command line prompt, you can access help in these ways:


- For a list of all the available commands in the current module, at the prompt type a question mark (?) and press <Enter>.
- For a description of a specific command, type `Help` followed by the name of the command. You can only get online help about a command related to the current module you are in.
- For general system information type `Information`. Specify the subject or type ? and the available subjects are listed. This subject list is specific to the current module.

Typographical Conventions









The following typographical conventions are used throughout the documentation, both online and in the PDF documents.



TEXT

| Convention | Definition |
|---------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Forward arrow symbol → | The forward arrow symbol → instructs you to select a series of menu items in a specific order. For example, Tools → Options is equivalent to: From the Tools menu, select Options . |
| Boldface font | A boldface font indicates that the given word(s) are shown that way on a toolbar button or as a menu selection. For example, if you are told to select a menu item in a particular order, such as Tools→Options , or to click Save . |
| <i>Italic</i> font | An <i>italic</i> font in the body of the text indicates the introduction of important terminology. Expect to find an explanation in the same paragraph or elsewhere in the guide. |
| COMMAND | For features in Thermo-Calc that use Console Mode (i.e. the command line), this font and all capital letters indicates that this is a Console Mode COMMAND. Examples of how you can use a command are written with code font. For example: Use DEFINE_ELEMENTS followed by a list of the elements that you want in your system. (To list the elements that are available in your current database, use LIST_DATABASE and choose Elements). |
| HELP | Text in blue and underline and a page number is a link to another topic in the current or referenced guide. Command names are often also topics. Clicking the link takes you to more detail about a particular command or subject in the PDF or documentation set. |
| <Enter> | Text with <angle brackets> indicates a keyboard entry. Usually to press <Enter> (or Return) or to use a series of keys such as <Ctrl + S>. |
| code and code bold | A code font shows a programming code or code example. The code bold font highlights the entry. |
| click vs press | In general, you <i>click</i> with the mouse to perform an action on the screen (e.g. click Save) and you <i>press</i> keys on a keyboard to enter a set of commands (e.g. press Ctrl+S). |

| Convention | Definition |
|------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| |  <p>When working in Console Mode, you can use keyboard shortcuts. Sometimes a window opens where you have the option to Save, Cancel or Open a file, for example. In these cases the instructions might say <i>click</i> Save, whereas you would need to <i>press</i> the applicable keys to perform the action.</p> |

ICONS

| Convention | Definition |
|----------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Important |  <p>Provides important information. It is recommended that you read the text or follow the link.</p> |
| Note |  <p>The information can be of use to you. It is recommended that you read the text or follow the link to more information.</p> |
| Also see |  <p>Go to the link or guide to see more general information about the topic being discussed. Usually includes both text and a link.</p>  <p>The small blue arrow is used when there is one (sometimes two) cross reference and no text describing the link. Often used in settings pages to link you to accompanying theory or extra detail.</p> |
| Tip |  <p>This is general information that can be of use but is not required knowledge.</p> |
| Examples |  <p>Go to the example collection to learn more.</p> |
| Console Mode |  <p>This note relates specifically to something in Console Mode.</p> |
| Graphical Mode |  <p>This note relates specifically to something in Graphical Mode.</p> |

| Convention | Definition |
|----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Diffusion Module |  This indicates that the information relates to the add-on Diffusion (DICTRA) Module. |
| Precipitation Module |  This indicates that the information relates to the add-on Precipitation Module. |

Database Files

In this section:

| | |
|-----------------------------------------------------------------------------|----|
| About the Database Files | 31 |
| Database Installation Folder | 32 |
| About Cached Database Files | 33 |
| Editing the Database Initialization File or Unencrypted Database File | 34 |
| Database Checker | 35 |

About the Database Files



["Database Manager User Guide" on page 1](#)



Go to the [Thermo-Calc website](#) for links to all the current database information sheets.

Encrypted vs Unencrypted Database Files

Any licensed databases purchased from Thermo-Calc Software are encrypted in files with the extension `.TDC`; these files cannot be edited. These are referred to as *encrypted databases*.

Unencrypted databases have the file extension `.TDB` and can be edited. For example, PURE5 or PG35 (the free databases) or a user-defined database file. If you plan to edit any of these files.



["Editing the Database Initialization File or Unencrypted Database File" on page 34](#)

Database Initialization File

The *database initialization file* is called `tc_initd.tdb`. Individual licenses are still required to use each database.

The file is used differently by the program depending on whether you are working with databases in Console Mode or Graphical Mode. For this reason, editing the file can be problematic if you don't understand the differences.



["About Cached Database Files" on page 33](#) and ["Editing the Database Initialization File or Unencrypted Database File" on page 34](#)

User Database Files

A user-defined database is considered to be an unencrypted database because you can make changes to it.

In Graphical Mode you can add user databases via the **Options → Graphical Mode → System definer** window. Once you have added the user database it is available from the database list in the System Definer Configuration window.



["Global Settings: System Definer" on page 41](#) to add a user database.

In Console Mode, users may decide to add their own user-defined database to the database initiation file, which then makes it available in the Console window. If you plan to edit this file.

▶ ["Editing the Database Initialization File or Unencrypted Database File" on page 34](#)

Custom Databases: GES5 and GES6 Calculation Engine Version

As of Thermo-Calc version 2019b, the default calculation engine is set to GES6. For custom database users, you may sometimes see messages in the log indicating that additional preparation is being done by Thermo-Calc prior to a calculation. The preparation is carried out automatically; it is usually fast and only needed the first time a custom database is used after a modification. While databases with warnings are tolerated, databases that contain errors can only be loaded by GES6 after the errors are corrected.

The Database Checker tool uses the same parser as GES6 and can be used to verify the consistency and correctness of databases during development, before the databases are actually used.

▶ ["Database Checker" on page 35](#)



To globally set the default from GES6 back to GES5, go to the **Tools → Options** → ["General" on page 37](#) tab and click **Version 5** for the *Preferred Gibbs Energy System* setting. The ["SET GES VERSION" on page 118](#) Console Mode command is used to change GES versions for a single Thermo-Calc session.








Contact Thermo-Calc Software AB at info@thermocalc.com for more information about the changes or if you encounter any issues you think are related to the new version of the calculation engine.

Database Installation Folder

The standard Thermo-Calc databases and the database initialization file `tc_initd.tdb` are located in a subfolder to the Thermo-Calc installation. For example, in a Windows Standalone installation, you can find these in a folder called **data** where the file path is `C:\Program Files\Thermo-Calc\<version>\data`.

> This PC > OS (C:) > Program Files > Thermo-Calc > <version> > data

| Name | Type |
|-----------------------------------------------------------------------------------------------------------|----------------------|
|  tc_initd | Thermo-Calc TDB file |
|  STANDARD_DB_CLASSES.BIN | BIN File |
|  TCTI2 | File folder |
|  TCTI1 | File folder |
|  TCSLD3 | File folder |

About Cached Database Files



This is applicable to Graphical Mode.



Also see Global Settings ["General" on page 37](#) where you can set the default database directory path. There is also an option to clear the database cache, which may be helpful if you are having issues.

The first time you open a database in Graphical Mode it can take a little while for it to load, especially if it is one of the large databases such as TCFE or TCNI. However, the next time the database opens quickly because now the databases are cached, or stored, in Graphical Mode.

Think of a cache as an intermediate storage area. Once a database cache is established the file made easily accessible, even if you close the software program. It is the same concept as when you load a web page for the first time. The next time the page opens faster. This is also how it works for the databases in Thermo-Calc Graphical Mode.

Thermo-Calc caches the database files, both encrypted and unencrypted types, at two points –when you first open a database, sometimes called an *in-memory cache*, and then later as a *disk-based cache*.. The disk-based cache is what speeds up database loading and it is at this point that Thermo-Calc refers to the database initialization file for information. The disk-based cache uses a lookup key to find the abbreviated database name (e.g. TCFE or TCNI) contained in this initialization file.



It is important to understand the way databases are cached in Graphical Mode to ensure best practices for those who also use Console Mode, especially if the database initialization file is edited. If you plan to edit this file, see [Editing a Database Initialization File](#) or [Unencrypted Database File](#) for important information.

Editing the Database Initialization File or Unencrypted Database File

Some advanced users may decide to edit the database initialization file, for example to reorder the list of encrypted databases displaying in the Console window or to add their own user-defined database for use in Console Mode. It is important to understand that changes to this file impact the database caching process used in Graphical Mode.

▶ ["About the Database Files" on page 31](#)

▶ ["About Cached Database Files" on the previous page](#)

The following recommendations are also applicable if you edit an unencrypted database file, which includes user databases and free databases such as PURE5 or PG35.

Best Practice Recommendations

▶ ["Database Installation Folder" on page 32](#)

If you edit the database initialization file (tc.initd.tdb in Windows or initd.tdb in Mac and Linux), then:

- If a user database is added to the file, it is subject to the same caching as the encrypted databases. This means that further changes (to the user database) will not be detected when you are working with databases in the System Definer in Graphical Mode.

If you have a user database, which is subject to regular updates, then:

- If you make changes to a user database, you then need to clear the cache.
- It is recommended that you create a separate directory to store unencrypted database files.

If you edit an unencrypted database file included with the installation (such as the PURE5 and PG35 files):

- Do not edit the file in the installation folder. Instead make a local copy and load it into the application as a user database.

Database Checker

The Thermo-Calc software package includes a program to check that the syntax of unencrypted database files is correct. The program applies the syntax rules set out in the *Database Manager User Guide* and reports errors and issues warnings. This program is intended for advanced users who develop and manage databases.



Thermo-Calc accepts deviations from these syntax rules. This means that a database can work even if the Database Checker reports errors and warnings. For example, an error is reported if an abbreviated phase name is found, but phase name abbreviations are accepted by Thermo-Calc and its add-on modules.

The executable **DatabaseChecker** file is found in the Thermo-Calc home directory. The program can also be launched by selecting **Tools→ Database Checker** from the main menu.

▶ ["Database Manager User Guide" on page 1](#)

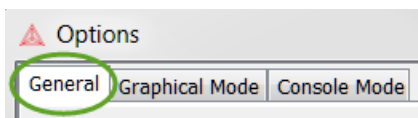
Changing Global Settings

In the **Options** window (select **Tools → Options**) you can globally set general settings for Graphical Mode as well as default settings for any new activities for both Graphical Mode and Console Mode.

In this section:

| | |
|------------------------------------------------------------|----|
| General | 37 |
| Graphical Mode - Default Units | 39 |
| Graphical Mode: Activities | 40 |
| Global Settings: Graphical and Console Mode Plotting | 47 |
| Global Settings: Console Mode Default Appearance | 54 |

General



These settings are for both Graphical Mode and Console Mode. To open this window, from the main menu select **Tools → Options**.

Tooltips enabled

Select whether to turn on tooltips information. By default the **Tooltips enabled** check box is selected. This displays a small text box when you hover the cursor above some buttons or other items.

Localization

To change the GUI language from the **Localization** list choose **English** (the default), **Swedish**, **Spanish**, **German**, **Russian**, **Chinese**, **Japanese** or **French**.

Look and feel

To change the **Look and feel** of the GUI layout, choose **Windows** (the default), **Metal**, **Nimbus**, **CDE/Motif** or **Windows Classic**.

Log level

Select the level and type of information to display in the **Event Log** window using the **Log level** slide bar. Choose from a **Debug**, **Info**, **Warning** or **Error** level of detail.

Database directory

In the **Database directory** field, specify the path to the directory that contains the **data** directory. This is where the Thermo-Calc database directory called **data** is located. Do not specify the path to where the database files are found (that is, in the **data** directory).

Modifying the Database Directory Path (Graphical Mode Only)



Important Note: Database Directory Path (Graphical Mode only)

When you open a database for the first time, it is stored in a cache (an intermediate storage area), that is maintained even if you close the program. This improves the speed of loading the next time you open that database. The cache is used for all databases that are listed in the database initialization file, typically all the standard databases that are included with Thermo-Calc.

If you modify your own user-defined database, or if you choose to edit an unencrypted database, it is recommended that you create a separate directory to store these database files. This way the most recent version of the user-defined or edited databases are loaded into the program when the System Definer is performed.

► ["About the Database Files" on page 31](#)

Model directory

This is where the predefined and custom property models are saved and stored by default. Click **Modify** to open the default folder or to create a custom folder for your own models.



All property models (whether these are predefined or custom models) must be located in a subdirectory of the property model directory. For that reason it is recommended that you do not change the directory location.



See ["Property Model Calculator" on page 75](#) for information about using the predefined models. Also see "Creating a New Property Model" in the *Property Model Development Framework Guide* for details about creating a custom model.

Check update interval

From the **Check update interval** list, choose not to check (**Do not check**, the default) or **On startup**. You can also manually check for updates – choose **Help→Check for Updates**.

Preferred Gibbs Energy System

► ["About the Gibbs Energy System \(GES\) Module" on page 36.](#)

Use this setting to globally set the default GES version to be either GES6 (the default) or GES5)

This setting is useful if you are using the PARROT module (optimization), POURBAIX module (aqueous solutions) or if you have a custom database that is not compatible with GES6. The ["SET GES VERSION" on page 118](#) Console Mode command can also be used to change GES versions for a single Thermo-Calc session.



Contact Thermo-Calc Software AB at info@thermocalc.com for more information about the changes or if you encounter any issues you think are related to the new version of the calculation engine.

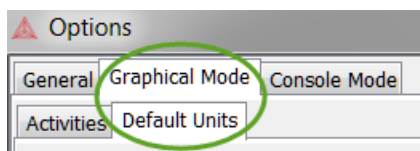
RESET ALL SETTINGS AND THE DATABASE CACHE TO DEFAULTS

Click **Factory reset** to reset all the settings to the original defaults, including clearing the database cache. The changes are applied when Thermo-Calc is restarted. This may be useful when there are several versions of Thermo-Calc installed and there are conflicts between settings or loading databases becomes problematic. See ["About Cached Database Files" on page 33](#).

Reset to original settings

In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to expand the window to view the button.

Graphical Mode - Default Units



To open this window, from the main menu select **Tools → Options** and click the **Default Units** tab.

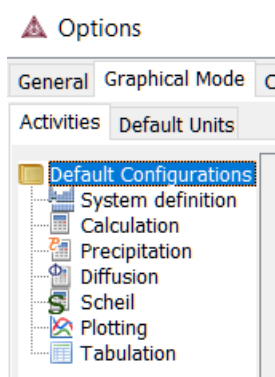
Reset to original settings

In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to expand the window to view the button.

| Setting | Options |
|-------------|---------------------------------------------|
| Temperature | Kelvin (the default), Celsius or Fahrenheit |
| Pressure | Pascal (the default), Atmospheres or Bar |

| Setting | Options |
|-------------|---------------------------------------------------------------------------------|
| Amount | Mole (the default), Gram, Kilogram or Pound |
| Composition | Mass percent (the default), Mole percent, Mass fraction or Mole fraction |
| Energy | Joule (the default), Calorie or Electron volt |
| Volume | Cubic meter (the default), Cubic decimeter or Cubic centimeter |
| Density | Kilogram per cubic meter (the default) or Gram per cubic meter |
| Entropy | Joules per Kelvin (the default), Calorie per Kelvin or Electron volt per Kelvin |
| Length | Meter (the default), Micrometer or Nanometer |
| Time | Seconds (the default), Hours or Days |

Graphical Mode: Activities



To open this window, from the main menu select **Tools → Options** and click the **Activities** tab.

There are **System definition**, **Calculation**, **Precipitation**, **Diffusion**, **Scheil**, **Process Metallurgy**, **Plotting** and **Tabulation** settings windows.



For Plotting, the default settings are shared with the Graphical and Console Modes. Any changes you make also apply to the default settings on the **Console Mode → Plotting** tab in the **Options** window (and vice versa).

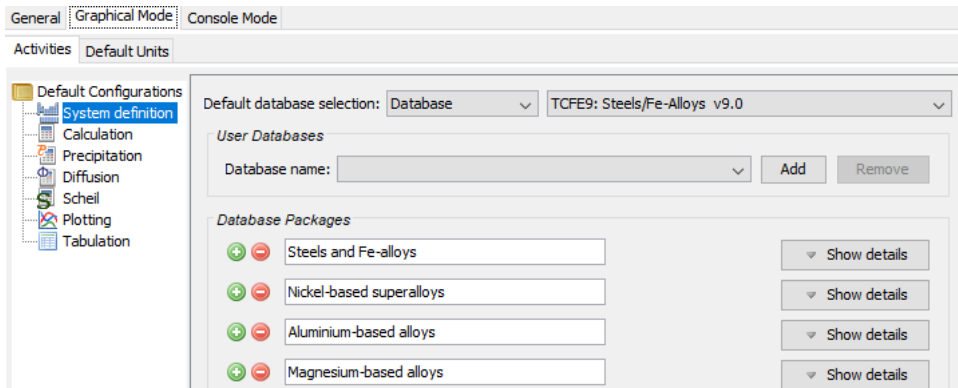


["Global Settings: Graphical and Console Mode Plotting" on page 47](#)

Global Settings: System Definer

When you create a new System Definer, the default databases are taken from these defaults. The database selections for each System Definer can then be configured individually. Once created, the specific (local) settings for a System Definer are not affected if you later make changes to the global defaults.

To open this window, from the main menu select **Tools → Options** and click the **Activities** tab. Then click **System definition**.



▶ ["System Definer" on page 36](#)

▶ ["Creating a Database Package" on the next page](#) and ["Clearing a Database Package Message" on page 43](#)

Default database selection

Choose to define a **Database** or a **Database package**.

If you choose **Database**, then select the default installed database to use globally for all System Definer nodes. For example, choose **TCFE9** or **TCNI8**.

If you choose **Database Package**, select an option from the list. These Database Packages are defined in *Database Packages*.

User Databases



Database name

Click the **Add** button to add a custom database. After you have added the user database it is available from the list to choose as the default.

Once a user database is added to the **Database name** list, you can also click the **Remove** button to delete it from your project.

Database Packages

Based on the installed databases, there are also default Database Packages available.

Create and remove **Database Packages** by clicking the **Add a database package**  button or **Remove this database package**  button.



The addition or removal of a database package does not take effect until a new System Definer node is defined.

Click **Show details** to display the list of databases included with the package. Click **Hide details** to only display the name of the package.





["Creating a Database Package" below](#)

Reset to original settings

In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to expand the window to view the button.

Creating a Database Package

1. From the main menu select **Tools → Options** .
2. Click the **Activities** tab and click **System definition**.
3. Under **Database Packages**, click the **Add a database package**  button.
4. Replace the default text with a name for the package, for example **My database package**.
5. Select a database from the **Choose database** list, for example, **TCFE9 Steels/Fe-Alloys**.
6. Click the **Add a database**  button and from the **Choose database** list, select another database, for example, **TCCU2 Cu-Alloys**
7. Click **OK**. The Database Package is now available to choose as the default for new System Definer activities.

Default database selection: Database Package ▼ Demo: Steels and Fe-alloys [FEDEMO, MFEDEMO] ▼

User Databases

Database name: Add Remove

Database Packages

☐ Demo: Steels and Fe-alloys

☐ My database package



The package is available for new System Definer nodes defined after adding the package.

System Definer 2

Package: ----- ▼

Magnesium-based alloys (TCMG4, MOBMG1)
 Ultra-high-purity silicon (TCSI1, MOBSI1)
 Solder alloys (TCSLD3, MOBSLD1)
 Copper based alloys (TCCU2, MOBCU2)
 Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO)
 Demo: Nickel-based superalloys (NIDEMO, MNIDEMO)
 Demo: Aluminium-based alloys (ALDEMO, MALDEMO)
 My database package (TCFE9, TCCU2)

Material

Material name:

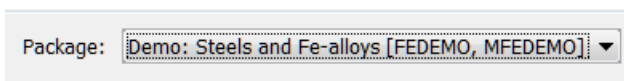
► ["Clearing a Database Package Message" below](#) and ["Global Settings: System Definer" on page 41](#)

Clearing a Database Package Message

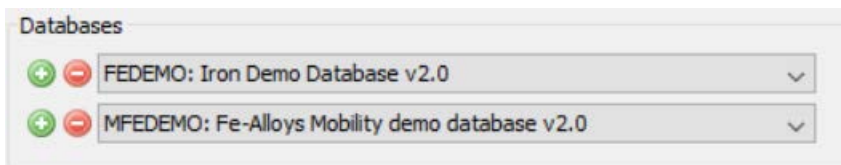
Sometimes when working on the System Definer Configuration window, you may add or delete Databases. If you originally added a Database Package, the addition or removal of a database means that the original package you selected does not now match the databases you are using. To clear the message *Selected databases and selected package may differ* and reset the databases you need to either:

- Change the newly added database back to the one that matches the database package, or
- Choose another package from the **Package** list, then select the package you want.

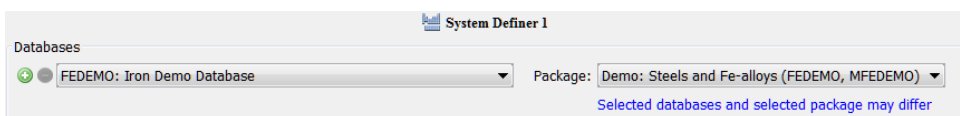
For example, from the **Package** list you select **Demo: Steels and Fe-alloys**.




This adds the **FEDEMO** and **MFEDEMO** databases.



If you add or remove **Databases**, in this example **MFEDEMO** is removed, then this does not match the **Package** and the message displays:



To clear the message, click the **Add a database**  button and from the **Choose database** list, select the database that belongs with the package, in this example, **MFEDEMO**. The message is cleared.

You can also choose another package from the list, which changes the databases, and then re-select the original package to reset the message.

► ["Creating a Database Package" on page 42](#) and ["Global Settings: System Definer" on page 41](#)

Global Settings: Equilibrium Calculator

When you create a new Equilibrium Calculator, its initial settings are taken from these defaults. The settings of each Equilibrium Calculator can then be configured individually. Once created, the specific (local) settings for an Equilibrium Calculator are not affected if you later make changes to the global defaults.

To open this window, from the main menu select **Tools → Options** and click the **Activities** tab. Then click **Calculation**.

► ["Options Tab Settings" on page 53](#)



You can reset the defaults. In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to expand the window to view the button.

Global Settings: Diffusion Calculator

When you create a new Diffusion Calculator, its initial settings are taken from these defaults. The settings for each Diffusion Calculator can then be configured individually. Once created, the specific (local) settings are not affected if you later make changes to the global defaults.

To open this window, from the main menu select **Tools → Options** and click the **Activities** tab. Then click **Diffusion**.

▶ ["Options Tab Settings" on page 121](#)

Reset to original settings

In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to expand the window to view the button.

Global Settings: Precipitation Calculator

When you create a new Precipitation Calculator, some of its initial settings are taken from these defaults. The settings for each Precipitation Calculator can then be configured individually. Once created, the specific (local) settings for a Precipitation Calculator are not affected if you later make changes to the global defaults.

To open this window, from the main menu select **Tools → Options** and click the **Activities** tab. Then click **Precipitation**.

▶ ["Conditions Tab Settings" on page 132](#)

Reset to original settings

In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to expand the window to view the button.

Global Settings: Process Metallurgy



The Material Manager is only available from this window. Use it to create material groups, as described below.

When you create a new **Process Metallurgy Calculator**, its initial settings are taken from these defaults. The settings for each Process Metallurgy Calculator can then be configured individually. Once created, the specific (local) settings are not affected if you later make changes to the global defaults.

To open this window, from the main menu select **Tools → Options → Graphical Mode** and click the **Activities** tab. Then click **Process Metallurgy**.

Except for the Material Manager, you can globally adjust the other settings, which are described for the ["Options Tab " on page 174](#).

Material Manager

▶ For more information see ["Working with the Material Manager" on page 176](#).

Use the **Material group** and **Material** lists to create and delete material groups, as well as delete material compositions that are saved from the Process Metallurgy Calculator.

- **Material group:** To create or delete a group, choose it from this list, e.g. **Steel** , **Slag** or **Gas**. The *Steel* group is simply a generic **Metal** group. You can create other user-defined metal groups and then these would also be listed here. Click **Create group** or **Delete group** as required to manage the list.
- **Material:** To delete a material, choose the group type then select the material composition to delete. For example, select the **Slag** material group, then choose the **Example Slag** material and click **Delete material** to remove it from all lists.

Reset to original settings

In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to expand the window to view the button.

Global Settings: Scheil Calculator

When you create a new Scheil Calculator, its initial settings are taken from these defaults. The settings of each Scheil Calculator can then be configured individually. Once created, the specific (local) settings for a Scheil Calculator are not affected if you later make changes to the global defaults.

To open this window, from the main menu select **Tools → Options** and click the **Activities** tab. Then click **Scheil**.

▶ ["Configuration Window Settings" on page 69](#)

Reset to original settings

In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to expand the window to view the button.

Global Settings: Tables

When you create a new Table Renderer, its initial settings are taken from these default settings. The settings of each Table Renderer can then be configured individually. Once created, the settings of a Table Renderer are not affected by changes in the default settings.

To open this window, from the main menu select **Tools → Options** and click the **Activities** tab. Then click **Tabulation**.

► ["Configuration Settings" on page 197](#)

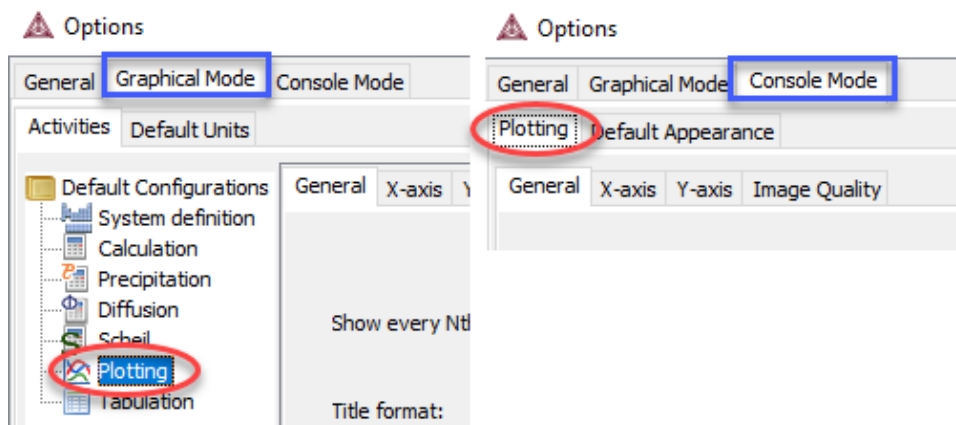
Reset to original settings

In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to expand the window to view the button.

Global Settings: Graphical and Console Mode Plotting



The default settings are shared with both modes. Any changes you make also apply to the default settings on the **Console Mode → Plotting** tab in the **Options** window (and vice versa).



Reset to original settings: In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to expand the window to view the button.

LOCAL PLOT PROPERTY SETTINGS

To make local changes to the appearance of a specific plot, in the **Results** window right-click a plot and select **Properties**. In the **Plot Properties** window a variety of settings can be made. These are the same settings as in the **Options** window.

You can also edit some properties for individual plot lines (the color, the line width and type, and whether data points are included). In the **Results** window, hover the mouse over a plot line. The crosshair cursor turns into a cursor resembling a pointing hand when it is over a line that can be clicked. Alternatively, hold down the <Ctrl> key while you move the cursor around the plot to only display it as a crosshair and prevent unintended edits.

GLOBAL CONFIGURATION (OPTIONS)

To globally configure the default settings for plotting, from the main menu select **Tools → Options**. You access the same settings either from the **Graphical Mode** or **Console Mode** tabs.

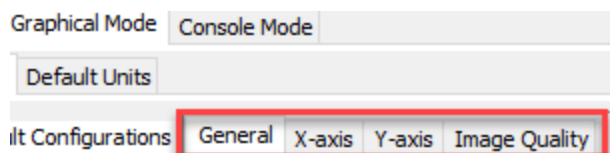
- Click the **Graphical Mode → Activities** tabs and then click the **Plotting** node in the tree, or
- Click the **Console Mode → Plotting** tabs.



When you create a new Plot Renderer, its initial settings are taken from these default settings. The settings can then be configured individually. Once created, the settings of a Plot Renderer are not affected by changes to the default global settings.

To configure the settings of an individual Plot Renderer rather than the default settings, right-click a plot in the **Results** window and select **Properties** from the menu.

The following global settings are available for both Console and Graphical Modes. Most of the settings are found on the **General** tab. Additional settings below for the **X-axis**, **Y-axis** or **Image Quality** tabs are indicated.



Titles, Legends and Labels

Title format and Label format

Select **Plain text** (the default) or **LaTeX formatted text**.



For **LaTeX formatted text** you can use the LaTeX math text to enter text. See ["ADD_LABEL_TEXT" on page 352](#) and ["Plot Labels " on page 234](#) for more details.

Show legend

Select the check box to include a legend on the plot. By default no legend is displayed.

Legend phase caption style

Choose **All**, **Constitution description** or **Ordering description**.



["About Legend Styles" on page 236](#)

Retain labels



Graphical Mode only.

By default the check box is selected. Plot labels are kept (retained) when plots are updated. It can be applied globally or locally to individual plots.

Show header



Console Mode only.

Click to select the **Show header** check box to display the basic details about the plot along the top. This includes the date and time the plot is generated, the database used and the properties.

Axis label format

This setting is available for both the X-axis and Y-axis tabs.

Choose either **Plain text** or **LaTeX-formatted text**.

Axis label font

This setting is available for both the X-axis and Y-axis tabs.

Click the **Modify** button to the right of the window to select a **Font name, Style, Size** and **color**.

Choose or enter a **Tick mark length** (**3** is the default). The defaults are to have the **Tick marks outside the chart** and to **Show tick labels**. Click to clear the check boxes as required.

Tick label font

This setting is available for both the X-axis and Y-axis tabs.

Click the **Modify** button to the right of the window to select a **Font name, Style, Size** and **color**

Fonts and Background Colors

Title font, Legend font, Label font, Header font

Click **Modify** to edit the Font Name, Style, Size and Color.

Legend background color, Background color, Canvas color, Border color,

Click **Modify** to choose a color or enter a specific color.

Lines and Grids

Show grid

Select the check box to include a grid on the plot. By default no grid is displayed.

Show every Nth tieline



Tielines are only applicable to phase diagrams.

Choose an integer value ranging from 0 to 99.

Color option (plot lines)

For the plot line colors, choose from the options in the list: **Legacy, Printer friendly, JFree**

chart, Pastel, Medium dark, Bright dark, Vivid or Earth.

This option is also available for specific plot lines. To change the color of an individual plot line double-click it in the Results window and use the color palette to define it or enter a specific color.

Border width

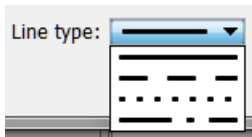
Choose a plot border width between **1** (thin, the default) and **10** (thick).

Line width

For the plot line width, choose from the options in the list. These options are also available for specific plot lines. To change an individual plot line width double-click it in the Results window.

Line type

This option is only available for individual plot lines. To change an individual plot line type double-click it in the Results window and choose an option from the list.



Data Points and Anchors

Show anchor

By default, an anchor between the label and the plot point is displayed.

Show data points

Click to select the check box to display the data points on the plot lines. This option is also available for specific plot lines. To show data points on an individual plot line double-click it in the Results window and select the check box.

Data points marker size

Choose the data point marker size between **1** (small) and **10** (large). The default is 3.

Plot Area Size

Plot area size

The **Fit the plot area size to the enclosing window** option is selected by default.

Click **Define the plot area size** to enter a **Plot area height** and **Plot area width (not applicable to triangular plots)**. The units are pixels and the size is kept as the size on the screen (96 dpi).

Image Quality

Image Quality

Choose the **Default file format**: **png** (the default), **gif**, **emf**, **pdf**, **ps**, **svg**, or **jpg**.



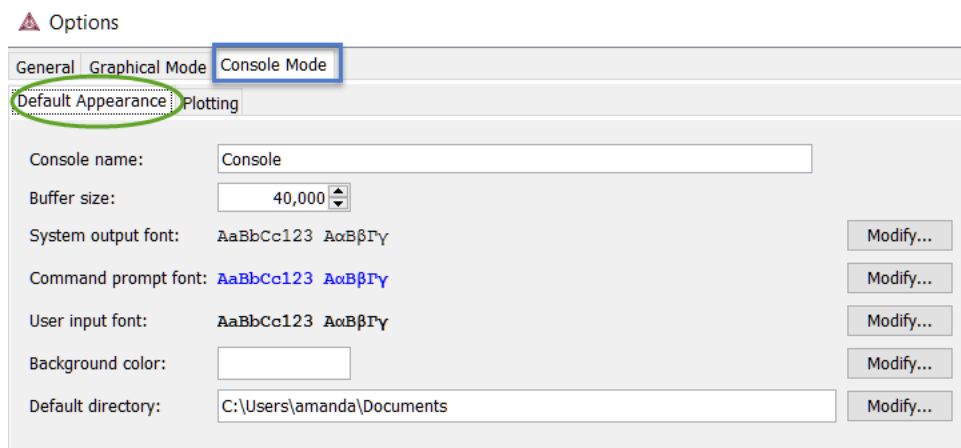
The following settings are only available for PNG and JPG.

To change the resolution of a PNG or JPG image, click to clear the **Use screen resolution** check box. Then enter a numerical value in the **Dots per inch (DPI)** field.

For JPEG files, you can also use the slider to choose a number between 0 and 1 for the **JPG quality**. The default is 0.9. The lower the number, the smaller the file.

Global Settings: Console Mode Default Appearance

To open this window, from the main menu select **Tools → Options**. To change the name, buffer size, fonts and colours for a specific Console window, right-click the label for that particular Console and select **Properties**.



Console name

The default is `Console` or enter another name to display.

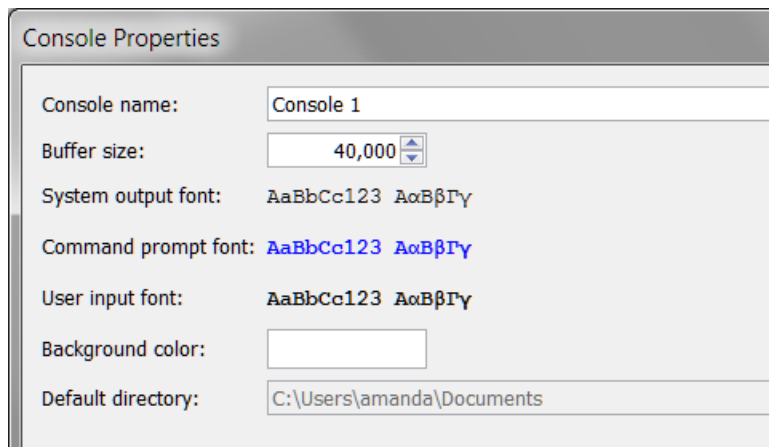
Buffer size

The default buffer size is 40,000.

INCREASING THE BUFFER SIZE

In Console Mode, sometimes the output overflows the window text buffer.

1. Right-click the Console tab header in the Console window (if this is the first Console tab, it is labeled **Console 1**).
2. Click **Properties**, and increase the **Buffer size** in the Console Properties window.



System output font

Click **Modify** to open the **Select Font** window and makes changes to the font type, style, size or color as required.

User input font

Click **Modify** to open the **Select Font** window and makes changes to the font type, style, size or color as required.

Command prompt font

Click **Modify** to open the **Select Font** window and makes changes to the font type, style, size or color as required.

Background color

Click **Modify** to open the **Select Color** window to choose a background color for the Console

Mode window where you enter commands.

Default directory

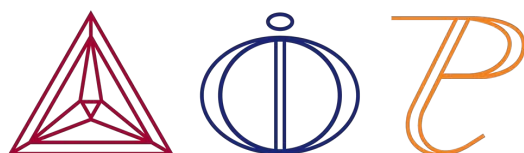
Set the default directory file path to where the various file types are saved.

Reset to original settings

In the lower corner of the window, click the **Reset to original settings** button to restore the original settings. You may have to expand the window to view the button.

Thermo-Calc User Guide: Graphical Mode

Thermo-Calc Version 2020a



Working in Graphical Mode

In this section:

| | |
|---------------------------------------------|---|
| The Graphical Mode Desktop Layout | 3 |
| Menu, Toolbar and Keyboard Shortcuts | 4 |
| Organizing the Windows on the Desktop | 6 |

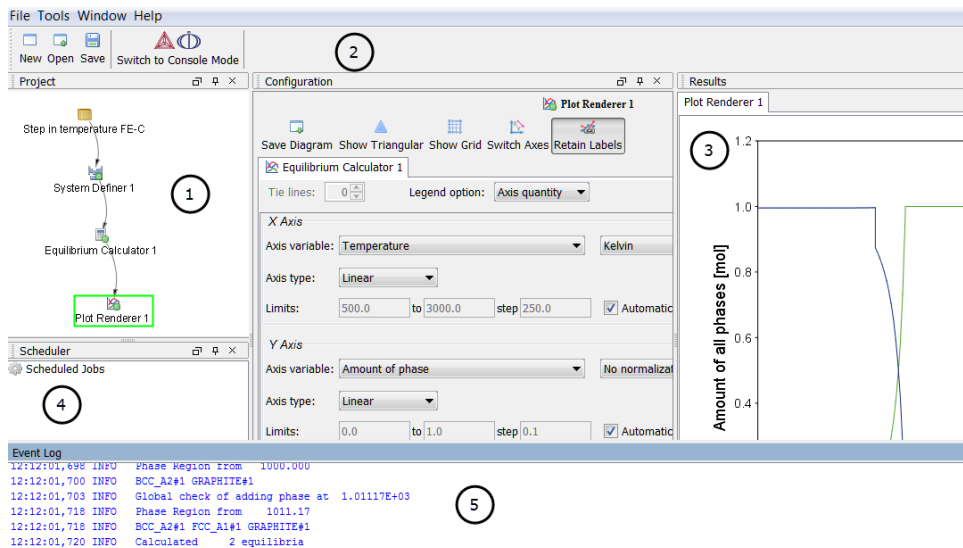
The Graphical Mode Desktop Layout

Open Thermo-Calc to view the default graphical user interface (GUI) layout for Graphical Mode.

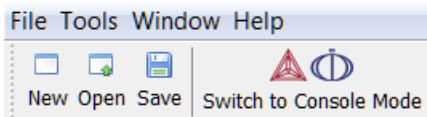
The windows are:

1. **Project:** Create, manipulate and navigate between the activities that make up a project. Click the **My Project** node to access the Quick Start wizard and a variety of templates.
2. **Configuration:** Shows the settings that can be configured for the currently selected activity.
3. **Results:** Shows the results of a calculation, either plotted as a diagram or displayed in table format. In this example, there is a Plot Renderer *tab* in the Results window.
4. **Scheduler:** Displays information about jobs, such as calculations, that are being performed or are scheduled to be performed. You can cancel scheduled jobs and if a job has failed, then you can view information about the error.
5. **Event Log:** By default this window is closed but it displays during calculation processes. You can always open it to view progress of calculations and to troubleshoot.

In this example, the **Results** window also has a **Plot Renderer** tab. You can also have a **Table Renderer** tab.



Menu, Toolbar and Keyboard Shortcuts




The **File** menu and toolbar are reserved for Graphical Mode but in Console Mode the **Tools**, **Window** and **Help** menus have the same options.



In Console Mode you use commands to access the other options, for example see ["Main Menu Commands" on page 15](#).

GRAPHICAL MODE MENU AND TOOLBAR OPTIONS

| Option | Description | Action (s) |
|--------------------------|-----------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------|
| New | Create a new project. | Click New on the toolbar Select File → New Project Windows: Press <Ctrl+N> Mac: Press <⌘N> |
| Open | Open an existing project. See "Saving and Opening Project Files" on page 21 . | Click Open on the toolbar Select File → Open Project Windows: Press <Ctrl+O>. Mac: Press <⌘O> |
| Save | Save a project. See "Saving and Opening Project Files" on page 21 . | Click Save on the toolbar Select File → Save Project Windows: Press <Ctrl+S>. Mac: Press <⌘S> |
| Save Project As | Save an existing project with a new name. | Select File → Save Project As Windows: Press <Ctrl+Shift+S> Mac: Press <⇧⌘S> |
| Switch to Console Mode | Launch Console Mode and the command prompt. | Click the button to exit Graphical Mode and open Console Mode. |
| Switch to Graphical Mode | Launch Graphical Mode to work with the GUI version. | Click the button to exit Console Mode and open Graphical Mode. |

| Option | Description | Action (s) |
|-------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------|
| Append Project | Combine two projects into one project file. See "Saving and Opening Project Files" on page 21. | Select File → Append Project Windows: Press <Ctrl+Shift+O> Mac: <⇧⌘O> |
| Exit | Exit the program. | In the upper right-corner of the program, click the X. Select File → Exit Windows: Press <Ctrl+Q>. Mac: <⌘Q> |
| Options | Change the global defaults for a variety of settings. See "Changing Global Settings" on page 36. | Select Tools → Options |
| Database Checker | Open the Database Checker, a program to check that the syntax of Thermo-Calc database files is correct. This is for advanced users who develop and manage databases. | Select Tools → Database Checker |
| Window menu | Highlight a specific window on the GUI | From the Window menu, select an option to refocus on that specific window. |
| Help | Open the online help system where you can browse or search all the Thermo-Calc documentation.  This does not require an Internet connection. The content is stored locally. | Press <F1> Select Help → Online Help |
| Video Tutorials | Open a link to the Thermo-Calc website where a variety of video tutorials are available. | Select Help → Video Tutorials |
| Examples Files | Open the examples folder based on whether you are in Console Mode or Graphical Mode. | Select File → or Help → Examples Files |
| Manuals Folder | Open the folder on your computer that has the PDF documentation and guides. | Select Help → Manuals Folder |
| Show License Info | Open the License Information window.  Also see "Displaying Thermo-Calc License Information" on page 13 and the <i>Thermo-Calc Installation Guide</i> | Select Help → Show License Info |
| Check for update | Check the Thermo-Calc Software website for updates to the software. | Select Help → Check for Updates |

| Option | Description | Action (s) |
|-----------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------|
| Request Support | Open a link to the Support page on the Thermo-Calc website. There are instructions about how to submit your question to the Support email: support@thermocalc.com | Select Help → Request Support |
| About | Includes the version number of the installed software and information about third party software licenses. | Select Help → About |

Organizing the Windows on the Desktop

The windows on the Thermo-Calc desktop can be fixed or free-floating. By default, most windows are fixed and open.

AUTO-HIDING A WINDOW

When a window is fixed it can also be set to auto-hide. Auto-hiding means that the window is minimized when you select another window. The minimized window is then shown either along the bottom or side of Thermo-Calc. A free-floating window is shown on top of the other windows and can be moved outside the frame of Thermo-Calc.







The **Event Log** window is set by default to auto-hide.



RESETTING THE DESKTOP LAYOUT

To return to the standard desktop layout, from the main menu, select **Windows → Reset Windows**.

FLOATING, HIDING AND MINIMIZING WINDOWS IN THE GUI

For each window you can rearrange, resize, minimize and close it. At the top right corner are the buttons listed in the table.

| Button(s) | Description |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------|
|   | Click to toggle on/off free-floating |
|   | Click to toggle on/off auto-hide. |

| Button(s) | Description |
|-----------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------|
|  | Click to minimize an open window that has auto-hide turned on. The window automatically minimizes if another window is selected. |
|  | Click to close the window. You can open the window again from the Window main menu. |

Projects and Activities

In this section:

| | |
|---------------------------------------------------|----|
| About the Activity Nodes | 9 |
| Graphical Mode Activity Node Workflow | 12 |
| Creating Activities and Successors | 13 |
| Cloning Activities and Trees | 14 |
| Moving Nodes in the Tree and Using the Grid | 15 |
| Node or Window Status Markers | 17 |
| My Project and Activity Menus | 18 |
| Saving and Opening Project Files | 21 |
| The Calculation Types in Graphical Mode | 23 |
| The Quick Start Wizard and Templates | 26 |

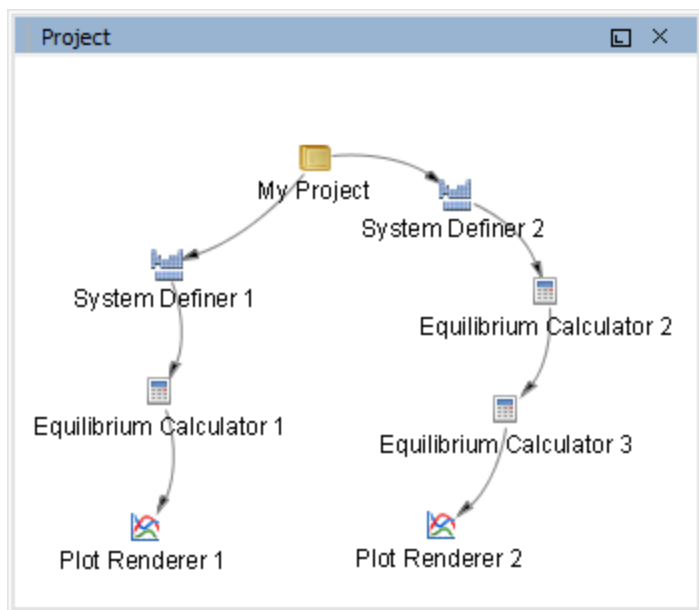
About the Activity Nodes

► ["Graphical Mode Activities vs Console Mode Modules " on page 7](#)

In a *project*, a set of linked activities is called a *tree*. A result calculated within a tree is fed as input into the next *activity* in the tree. Consequently, if you have an Equilibrium Calculator with another Equilibrium Calculator as its *successor*, the successor takes the calculation results of the *predecessor* as the starting values for its calculation. When working with activities in the Project window these are also referred to as *nodes* (or *activity nodes*) in the tree structure.

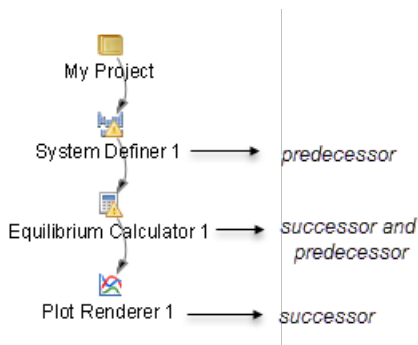
The example below shows a *My Project* node with two trees. In each tree, settings and calculation results are propagated downward until the calculation and the visualization of the results are completed in the *Plot Renderer* nodes.

The system definitions, settings and calculation results of the two trees are independent of each other.



Activity Successor and Predecessor Nodes

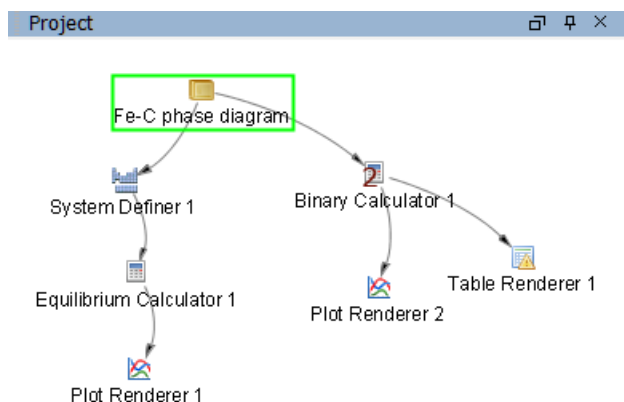
An activity node located below another activity node in a tree is referred to as that activity's *successor*. An activity located above another activity is called that activity's *predecessor*. A predecessor is performed before the predecessor's successors and its result is fed forward to any successor activities.



For example, to calculate and display a phase diagram, create a branch with three linked activities: A **System Definer** activity linked to an **Equilibrium Calculator** activity, which in turn is connected to a **Plot Renderer** activity.

See the example below that shows that **Binary Calculator 1** is a predecessor to the successors, **Plot Renderer 2** and **Table Render 1**.

You can determine the available successors by right-clicking a node in the **Project** window and choosing **Options** from the menus.




► ["Creating Activities and Successors" on page 13](#) and ["Cloning Activities and Trees" on page 14](#)

ACTIVITY NODE DESCRIPTIONS

The table below is a brief description of the activity types you work with in the **Project** window. When working with activities these are referred to as *nodes* in this documentation.

These are the project activity nodes available in Graphical Mode.

| Activity type | Description |
|-------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| "System Definer" on page 36 | Define a certain thermodynamic system and read it from file into memory. |
| "Property Model Calculator" on page 75 | Choose one or more General models and Steel models to predict and optimize material properties. You can evaluate models simultaneously over a range of compositions and cross plot the results. You can then conduct an uncertainty analysis and plot the results as either a histogram or as a probability plot. |
| "Equilibrium Calculator" on page 48 | Set thermodynamic conditions and define axis variables when a series of equilibrium calculations are to be performed in one or more dimensions. |
| "Precipitation Calculator" on page 129 | Set the conditions for, and perform, a precipitation calculation using the Precipitation Module (TC-PRISMA). You can also use this in DEMO mode with up to three components. |
| "Diffusion Calculator" on page 109 | Using the Diffusion Module (DICTRA), this activity is where you set the geometry, add one or more regions, enter grids and phases in the regions, and then enter compositions of phases. You can also use this in DEMO mode with up to three components. |
| "Process Metallurgy Calculator" on page 163 | This calculator allows for efficient setup of advanced calculations involving slag, metal and gas. Define the composition of a steel and slag system using material groups: one each for steel, slag and gas. |
| "Plot Renderer" on page 179 | Determine the layout of non-text based output. |
| "Table Renderer" on page 194 | Use it for text-based output. |
| "Binary Calculator" on page 60 | <p>Use it for some calculations involving two components only. It is like a combination of System Definer and Equilibrium Calculator activities with adaptations to simplify the configuration of calculations on binary systems.</p> <div>  <p>To perform this activity, you need a database designed for the Binary Calculator, such as the TCBIN database.</p> </div> |
| "Ternary Calculator" on page 63 | <p>Use it for some calculations involving three components. It is like a combination of System Definer and Equilibrium Calculator activities with adaptations to simplify the configuration of calculations on ternary systems.</p> <div>  <p>To get a reliable result you need a database that fully assesses binary and ternary systems.</p> </div> |
| "Scheil Calculator" on page 66 | Perform Scheil-Gulliver calculations (also known as Scheil calculations). A default Scheil calculation is used to estimate the solidification range of an alloy assuming that i) the liquid phase is homogeneous at all times and ii) the diffusivity is zero in the solid. However, it is possible to disregard the second assumption for selected components. |

| Activity type | Description |
|--------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------|
| "Experimental File Reader" on page 200 | Read experimental data files (*.EXP). This type of file contains information specifying a plotted diagram, written in the DATAPLOT graphical language. |

Graphical Mode Activity Node Workflow

You can set up a tree in the **Project** window (starting with the **My Project** node) and then perform all the activities at once, or create and perform one activity at a time.



You can also use the templates to add all the necessary activity nodes based on your simulation needs. See ["Creating a Project from a Template" on page 30](#).

The typical workflow is to:

1. *Define a System:* Add a ["System Definer" on page 36](#) activity (in the **Project** window) where you select a database and the elements to have as system components (in the **Configuration** window).
 - To the **My Project** node, you can alternatively add and define a ["Binary Calculator" on page 60](#), ["Ternary Calculator" on page 63](#), or ["Experimental File Reader" on page 200](#) or ["Process Metallurgy Calculator" on page 163](#) activity node.
2. *Set up and run a calculation:* Add an ["Equilibrium Calculator" on page 48](#) activity (a successor to the **System Definer**), where calculation conditions are set (temperature, pressure, etc.). This is where axis variables are set to create a property or phase diagram. These settings are also made in the **Configuration** window. You can also add a ["Property Model Calculator" on page 75](#), ["Precipitation Calculator" on page 129](#), ["Diffusion Calculator" on page 109](#) or ["Scheil Calculator" on page 66](#) to the System Definer.

▶ ["Property Model Calculator Workflow" on page 75](#)
3. *Visualize the results:* Add either a ["Plot Renderer" on page 179](#) or a ["Table Renderer" on page 194](#) activity in the **Project** window. When calculated, this creates a plot or table in the **Results** window. The results are shown in a **Plot Renderer** or a **Table Renderer** tab.



You need to **Perform** a Plot Renderer or a Table Renderer activity to visualize the calculation results from an Equilibrium Calculator.

- ▶ ["About the Activity Nodes" on page 9](#)
- ▶ ["The Quick Start Wizard and Templates" on page 26](#)

Creating Activities and Successors

You can create a new activity in these ways:

- In the **Project** window, right-click an activity and choose **Create New Activity (My Project node only)** or **Create New Successor** (all other nodes).
- Select the activity you want to create from the submenu.
- At the bottom of the **Configuration** window, click **Create New Activity** or **Create New Successor** and select the activity to create.
- Use the **Templates** or the **Quick Start Wizard** (click the **My Project** node and select templates from the **Configuration** window) to quickly add a set of activity nodes to the tree.

| Activity | Possible Predecessors | Possible Successors |
|-------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------|
| My Project | None; this is the first node of the tree structure. You can add activities using the Quick Start wizard or templates. ▶ "The Quick Start Wizard and Templates" on page 26 | System Definer, Binary Calculator, Ternary Calculator, Process Metallurgy Calculator, Experimental File Reader. Also choose templates from this level. |
| "System Definer" on page 36 | My Project, System Definer | Property Model Calculator, Equilibrium Calculator, Precipitation Calculator, Scheil Calculator |
| "Experimental File Reader" on page 200 | My Project | Plot Renderer |
| "Binary Calculator" on page 60 | My Project | Plot Renderer, Table Renderer |
| "Ternary Calculator" on page 63 | My Project | Plot Renderer |
| "Process Metallurgy Calculator" on page 163 | My Project | Plot Renderer, Table Renderer |
| "Property Model Calculator" on page 75 | System Definer | Plot Renderer, Table Renderer |
| "Equilibrium Calculator" on page 48 | System Definer, Equilibrium Calculator | Equilibrium Calculator, Plot Renderer, Table Renderer |

| Activity | Possible Predecessors | Possible Successors |
|--------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------|
| "Precipitation Calculator" on page 129 | System Definer | Plot Renderer, Table Renderer |
| "Diffusion Calculator" on page 109 | System Definer | Plot Renderer, Table Renderer |
| "Scheil Calculator" on page 66 | System Definer | Plot Renderer, Table Renderer |
| "Plot Renderer" on page 179 | Equilibrium Calculator, Property Model Calculator, Binary Calculator, Ternary Calculator, Scheil Calculator, Process Metallurgy Calculator, Diffusion Calculator, Precipitation Calculator, Experimental File Reader | None |
| "Table Renderer" on page 194 | Equilibrium Calculator, Property Model Calculator, Binary Calculator, Scheil Calculator, Process Metallurgy Calculator, Diffusion Calculator, Precipitation Calculator | None |

Cloning Activities and Trees

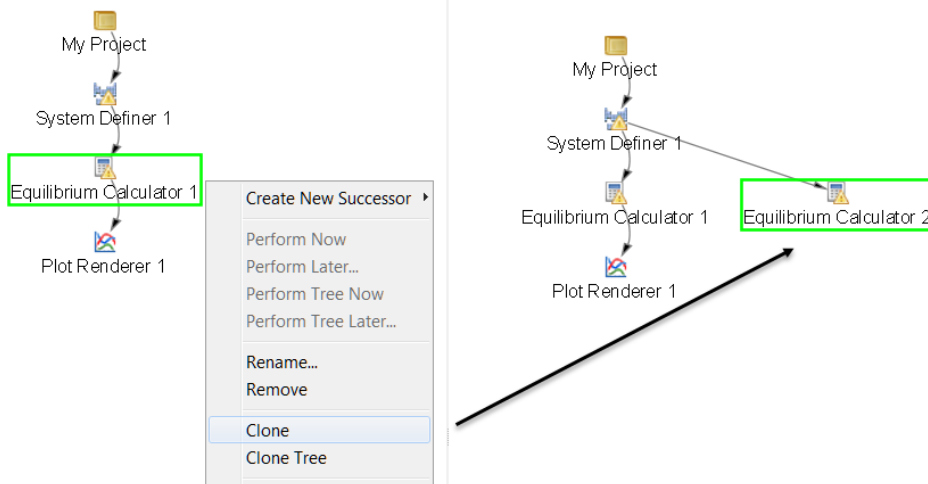
As described in ["Creating Activities and Successors" on the previous page](#), you can clone a single activity or the selected activity and all the activities that come after it (successors). The predecessor of the selected activity also is the predecessor of the clone.

Cloned activities are configured exactly like the activities that they were cloned from, and any results of calculations or plots are also cloned. To clone a selected activity, right-click the activity and select **Clone**.

For example, if you clone the Equilibrium Calculator in this project the result is an **Equilibrium Calculator 2** created as a successor to **System Definer 1**.

The following applies to clones.

- The new Equilibrium Calculator has the same settings for conditions, functions and options as its Equilibrium Calculator 1 clone.
- If the Equilibrium Calculator is already performed, then the calculation results are cloned.
- If the activity is a Plot Renderer or a Table Renderer, then the plot or table is cloned.
- If you want to clone all the successor activities that follow a selected activity, then right-click and select **Clone Tree** instead.



Cloning an Equilibrium Calculator activity node

ABOUT EQUILIBRIUM CALCULATOR CLONES AND SUCCESSORS

If you create an Equilibrium Calculator as a successor to another Equilibrium Calculator, then the successor inherits all the settings for conditions, functions and options from its predecessor. In this respect, it is similar to a clone.



The Equilibrium Calculator successor is different from a clone in that it does not inherit any calculated results and it is a successor to the Equilibrium Calculator instead of a successor to its predecessor.

The calculated result from an Equilibrium Calculator that is the predecessor to another Equilibrium Calculator is the starting value for the latter's calculation. The clone of an Equilibrium Calculator on the other hand, does not receive any data as input from the Equilibrium Calculator that it is cloned from.

Moving Nodes in the Tree and Using the Grid

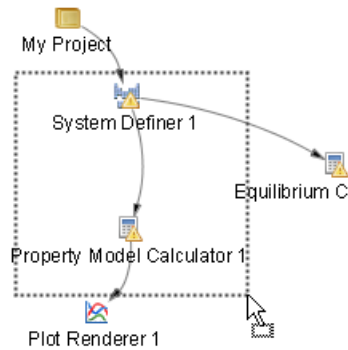
In the **Project** window, you can work with the activity nodes in these ways.

SELECT AND MOVE INDIVIDUAL NODES

- Click an activity node to *select* it.
- To move activities, click and hold the activity node and move the cursor.

SELECT SEVERAL NODES AT A TIME

-
- To select several activity nodes, hold down <Ctrl> while clicking on each node you want to select.
 - Click and hold the mouse button and draw a square around the activity nodes to select. Both the name and the icon that represents an activity must be within the square.



APPLY AUTO LAYOUT

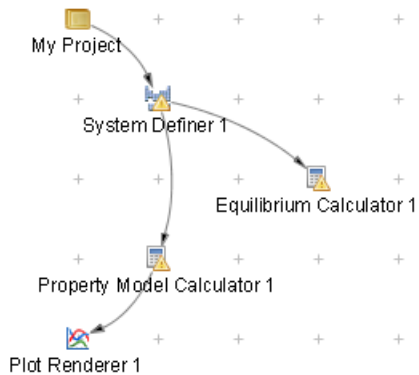
In the **Project** window, right-click anywhere and choose **Apply Auto Layout** from the menu. The nodes and the tree default to the center of the Project window.

SHOW GRID AND SNAP TO GRID

To show a grid of light-grey cross-hairs overlaid on a project, click **Show Grid** in the toolbar. Click the button again to turn the grid off. Or right-click in the **Project** window and select **Show Grid**.

Click **Snap to Grid** in the toolbar or right-click in the **Project** window and select **Snap to Grid** to automatically position each activity in the Project window at a cross-hairs point in the grid.

The Project window with the grid turned on and activity nodes moved from the default location. These nodes are snapped to the grid.







Node or Window Status Markers





Status markers indicate whether an activity is ready to be performed, is being performed, or has been performed. The markers are overlaid on the activity nodes in the **Project** window. The status markers are displayed on a **System Definer** node.

► ["About the Activity Nodes" on page 9](#)

STATUS MARKER DESCRIPTIONS

Node Status Markers for the Project and Scheduler Windows

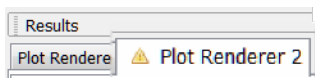
| Window | Status marker | Description |
|----------------|-------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------|
| Project window |  | No status marker means the activity is ready to be performed (it has not been performed). |
| |  | A yellow triangle means the activity cannot be run. The necessary configurations for the activity may not be set or other prerequisites are not met. |
| |  | A green disc means the activity is performed. |
| |  | A red circle with a dial (a clock face) means the activity is currently being performed. |

| Window | Status marker | Description |
|------------------|-----------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|
| Scheduler window |  | No status marker means the activity (the job) is scheduled to be performed (the job has not started). |
| |  | A yellow triangle means there an error happened during the activity job. |
| |  | A green disc means the activity (the job) performed successfully. |
| |  | A green right-facing arrow means the activity (the job) is being performed. |

RESULTS WINDOW STATUS MARKER

If you have plotted a diagram and then modify something in the tree that the Plot Renderer is associated with, then a notification —an exclamation mark enclosed in a yellow triangle— is shown in the Plot tab.

► ["Node or Window Status Markers" on the previous page](#)



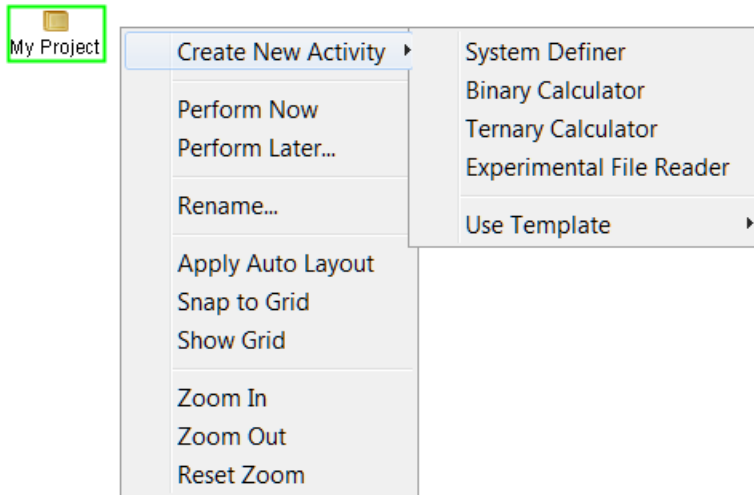
My Project and Activity Menus

When working in the Project window you can right-click nodes to open menus with the available actions. For example, click the **My Project** node to open the menus. Most nodes in the tree have a common menu with differences due to placement in the tree and the activity type.

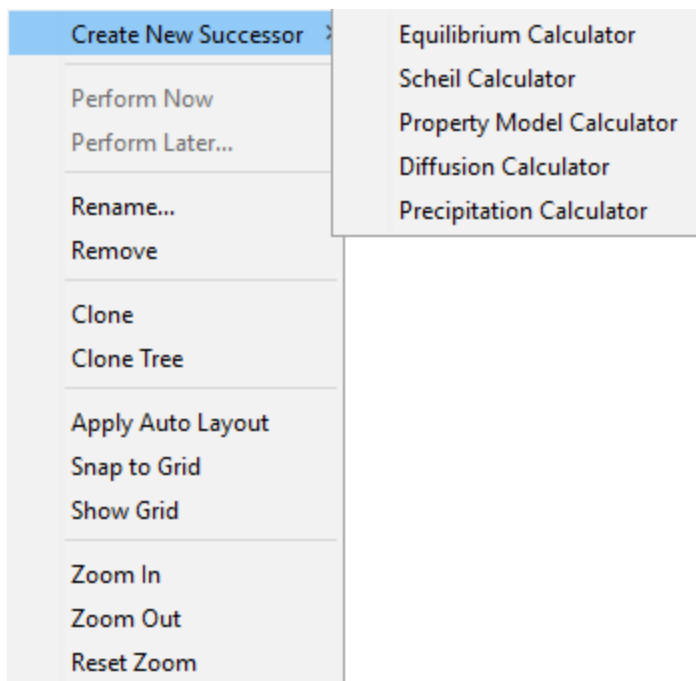
► ["About the Activity Nodes" on page 9](#)

MENUS





My Project Node





Activity Node



MENU OPTIONS FOR ACTIVITY NODES

| Option | Description | Action (s) |
|------------------------------------|-------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Create New Activity | Add System Definer, Binary Calculator, Ternary Calculator, Process Metallurgy Calculator, and Experimental File Reader nodes. | Right-click My Project and from the Create New Activity menu choose an option.  "Creating Activities and Successors" on page 13 |
| Create New Activity → Use Template | Choose from the available templates to use the Wizard or add predefined nodes. | Right-click My Project and from the Create New Activity → Use Templates menu choose an option. The templates are also available on the Configuration window, which you can access by clicking the My Project node, or from the Window menu.  "Creating a Project with the Quick Start Wizard" on page 28 or "Creating a Project from a Template" on page 30 |
| Create New Successor | Add a successor to the selected node. | Right-click the System Definer , any Calculator node or the Experimental File Reader . Then from the Create New Successor menu choose an option.  "Creating Activities and Successors" on page 13 |
| Add a Predecessor | Add a predecessor to the selected node. | Right-click a node to add a predecessor to it (when available). |
| Perform Now or Perform Later | Perform a calculation or create a plot or table immediately, or schedule it for a time in the future. | Right-click any node.  "Using the Scheduler" on page 202 |

| Option | Description | Action (s) |
|-------------------------------|-------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Rename | Change the name of the node. | Right-click any node. |
| Remove | Delete the selected node from the tree. | Right-click any node except My Project. |
| Clone | Duplicate the selected node and add it to the same tree. | Right-click any node except My Project.  "Cloning Activities and Trees" on page 14 |
| Clone tree | Duplicate a tree and add it to My Project. | Right-click any node except My Project. |
| Apply Auto Layout | Apply an automatic layout to the nodes in the tree. | Right-click any node. |
| Snap to Grid | Snap a node to align it with the grid. | Right-click any node.  "Moving Nodes in the Tree and Using the Grid" on page 15 |
| Show Grid | Turn the grid on or off in the Project window. | Right-click any node. |
| Zoom In, Zoom Out, Reset Zoom | Zoom in and out of the Project window or reset the zoom to the default. | Right-click any node. |

Saving and Opening Project Files

Thermo-Calc Graphical Mode uses project files with the file name suffix `.tcu`. The add-on Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA) also use the same file format in Graphical Mode.

Saving a Project File

To save your project and all its settings and results, on the toolbar click **Save**. Select to **Include calculated results in the project file** (the default) as required.

Appending a Project

You can only have one project file open at a time in any one instance of Thermo-Calc. However, you can attach (*append*) the trees from additional project files to the topmost **My Project** node. To append an additional project file in this way, from the main menu select **File → Append Project** and open a project file.

-
- ▶ ["Saving and Printing the Output \(Graphical Mode\)" on page 205](#) and *Saving Tabulated Data* for the ["Table Renderer" on page 194](#)

Opening a Project File

There are different ways to open project files.

IN THERMO-CALC

- From the main menu select **File → Open Project**.
- On the toolbar, click the **Open** button or press <Ctrl+O> (Windows) or <⌘O> (Mac) on the keyboard. Then navigate to the file on your computer and click **Open**.

ON YOUR COMPUTER

- Navigate to the project file and double-click to open it. This launches a new instance of Thermo-Calc.

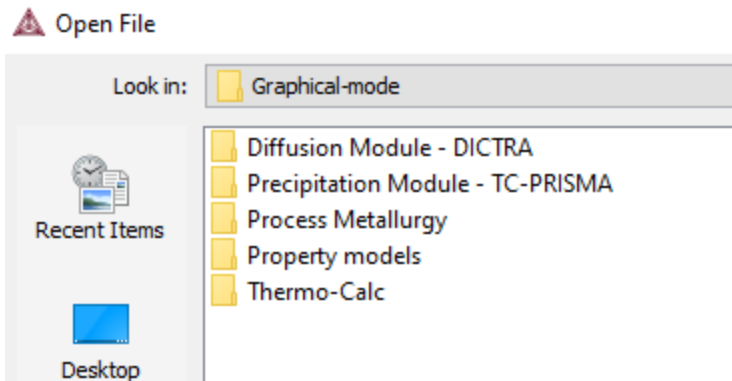
OPENING AN EXAMPLE PROJECT FILE FROM THERMO-CALC



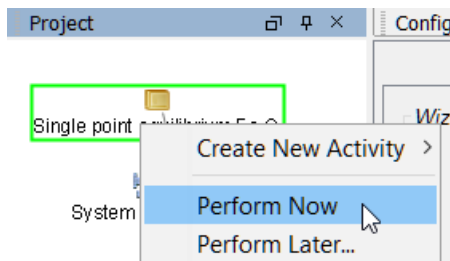
Some add-on module examples require additional licenses to run for more than three elements.

To open an example project file for Thermo-Calc and the add-on Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA):

1. Open Thermo-Calc.
2. Confirm you are in Graphical Mode. If not, click the **Switch to Graphical Mode** button.
3. From the main menu, select **File →** or **Help → Examples Files**.
4. The examples are divided into folders. Navigate to the folder and project file you want and double-click to open.



5. The Graphical Mode examples are stored without calculated results so you will want to run the example calculation and generate a plot or table. To do this, click the first node in the tree at the top of the **Project** window. Then right-click and select **Perform now**.



The Calculation Types in Graphical Mode

- ["Graphical Mode vs Console Mode: Calculation Types" on page 9](#)

Binary Calculator

The following calculation types are available for a Binary Calculator activity node:

- Phase diagram: To calculate in a defined multicomponent heterogeneous system, from one or more initial equilibria. A phase diagram is usually mapped within a specific space that is constructed by two (or more) defined independent mapping axis-variables.
- Gibbs energy curves: To calculate at a constant temperature over the whole composition range.
- Activity curves: To calculate at a constant temperature over the whole composition range.
- Phase fractions: To calculate as a function of temperature at a constant composition.

Diffusion Calculator

The following calculation types are available for a Diffusion Calculator activity node:

Detailed simulation of diffusion controlled reactions in multi-component systems. Diffusion calculations are done with the Diffusion Calculator. There are no calculation types you need to choose when setting up your simulation.

Equilibrium Calculator

The following calculation types are available for an Equilibrium Calculator activity node:

- Single equilibrium (no axes): To calculate a single point. The results from this calculation are displayed in the **Event Log**.
- One axis: To vary a quantity on the X-axis.
- Grid: Computes the equilibrium of each grid point in a two-dimensional grid.
- Phase diagram: To calculate in a defined multicomponent heterogeneous system, from one or more initial equilibria. A phase diagram is usually mapped within a specific space that is constructed by two (or more) defined independent mapping axis-variables.

Precipitation Calculator

The following calculation types are available for a Precipitation Calculator activity node:

-
- Isothermal: Precipitation simulation at constant temperature.
 - Non-isothermal: Precipitation simulation with user-defined temperature profile.
 - TTT diagram: Time-Temperature-Transformation diagram calculation.
 - CCT diagram: Continuous Cooling Transformation diagram calculation.

Process Metallurgy Calculator

The following calculation types are available for a Process Metallurgy Calculator activity node:

- Single: To calculate a single point. The results from this calculation can be displayed in the **Results** window using a **Table Renderer**.
- One axis: To vary a quantity on the X-axis.
- Grid: Evaluates two axis variables of the selected quantities in the specified range and number of steps.
- Uncertainty: Evaluates calculations where the values of the quantities are sampled from Gaussian distributions.

Property Model Calculator

The following calculation types are available for a Property Model Calculator activity node:

- Single: To calculate a single point. The results from this calculation are displayed in the **Event Log** or if a **Table Renderer** is used, in the **Results** window.
- One axis: To vary a quantity on the X-axis.
- Grid: Evaluates two axis variables of the selected quantities in the specified range and number of steps.
- Min/Max: Evaluates the property model(s) for all variations of the selected quantities at the given limits.
- Uncertainty: Evaluates the property model(s) where the values of the quantities are sampled from Gaussian distributions.

Scheil Calculator

The following calculation types are available for a Scheil Calculator activity node:

Simulate a non-equilibrium transformation or partial-equilibrium transformation (a Scheil-Gulliver solidification). Scheil calculations are done with the Scheil Calculator. There are no calculation types you need to choose when setting up your simulation.

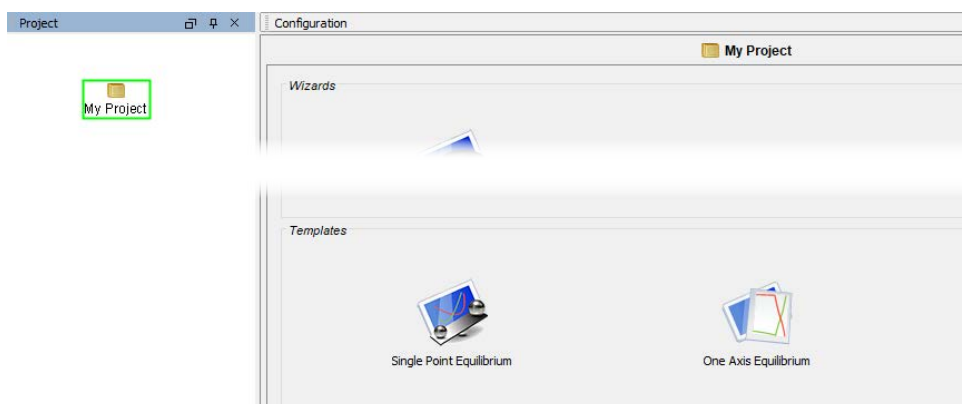
Ternary Calculator

The following calculation types are available for a Ternary Calculator activity node:

- Isothermal section: To calculate the ternary system for the whole composition range.
- Monovariant lines: To calculate the variation of the liquid compositions with temperature.
- Liquidus projection: The projection liquid surface and the monovariant lines are calculated over the given temperature range.

The Quick Start Wizard and Templates

Use the *Quick Start* wizard or a *Template* to create all the activities for a certain type of calculation. In the **Project** window click the **My Project** node to display the Quick Start and other templates in the **Configuration** window.



QUICK START WIZARD

Even before you understand how to work with Thermo-Calc projects, the Quick Start wizard helps you set up a project and run calculations in Graphical Mode. You can set up, calculate and visualize any of the following:

- Single point equilibrium
- One axis equilibrium

-
- Phase diagram
 - Scheil solidification simulation

▶ ["Creating a Project with the Quick Start Wizard" on the next page](#)

TEMPLATES

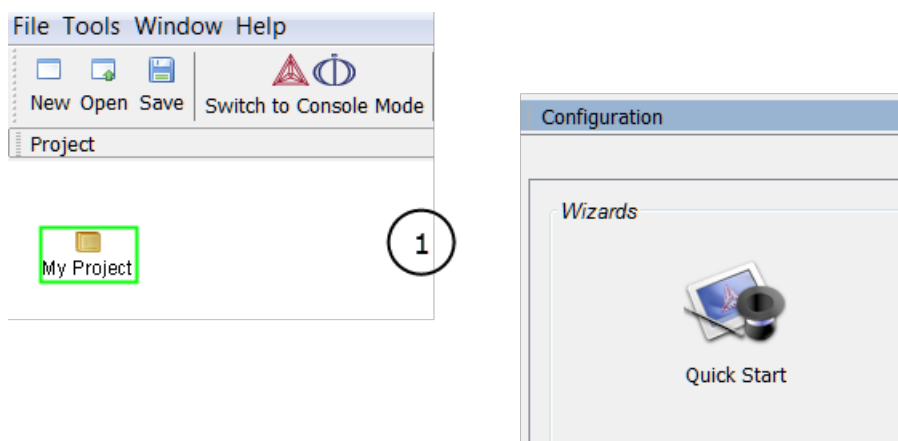
A variety of templates are available. You can add these from the **Configuration** window or by right-clicking the **My Project** node and selecting one from the **Create New Activity → Use Template** list:

- **Single Point Equilibrium:** Creates a project for calculating a single point equilibrium. The project consists of a System Definer, Equilibrium Calculator and a Table Renderer.
- **One Axis Equilibrium:** Creates a project for calculating a one axis diagram. The project consists of a System Definer, Equilibrium Calculator and a Plot Renderer.
- **Phase Diagram:** Creates a project for calculating a phase diagram. The project consists of a System Definer, Equilibrium Calculator and a Plot Renderer.
- **Scheil Solidification Simulation:** Creates a project for performing a Scheil calculation. The project consists of a System Definer, Scheil Calculator and a Plot Renderer.
- **Binary Calculation:** Creates a project for performing a binary calculation. The project consists of a Binary Calculator and a Plot Renderer.
- **Ternary Calculation:** Creates a project for performing a ternary calculation. The project consists of a System Definer, Ternary Calculator and a Plot Renderer.
- **Property Model Calculation:** Creates a project for a Property Model Calculator. The project consists of a System Definer, Property Model Calculator and a Plot Renderer.
- **Diffusion Simulation:** Creates a project for general diffusion simulations. The project consists of a System Definer, Diffusion Calculator and a Plot Renderer.
- **Precipitation Simulation:** Creates a project for simulating the evolution of particle size distributions. The project consists of a System Definer, Precipitation Calculator and a Plot Renderer.
- **Steel Library - TTT:** Creates a project for a steel package. The project consists of a System Definer, Property Model Calculator and a Plot Renderer.
- **Process Metallurgy:** Creates a project to allow for calculation and efficient setup of advanced calculations involving slag, metal and gas.

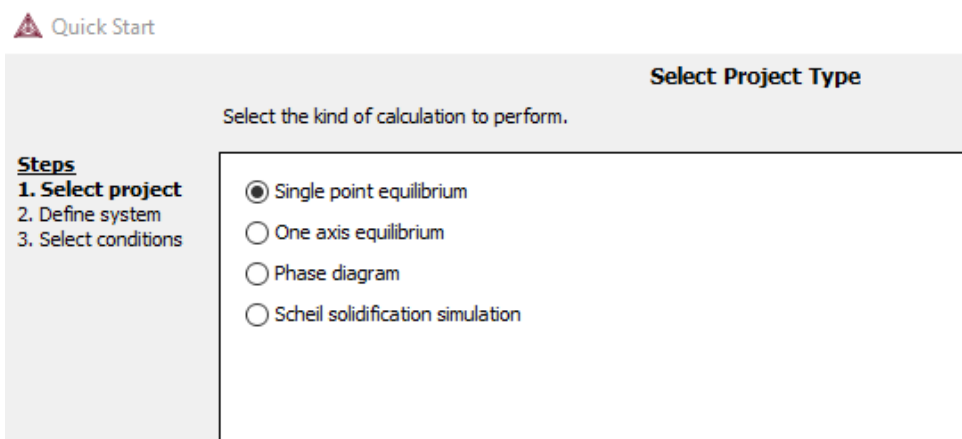
Creating a Project with the Quick Start Wizard

To set up, perform and visualize a calculation using the Quick Start wizard:

1. In the **Configuration** window click **Quick Start**. If you cannot see the **Quick Start** button, first click **My Project** in the **Project** window.



2. In the **Select Project Type** window click to select the type of calculation to perform. **Single point equilibrium**, **One axis equilibrium**, **Phase diagram** or **Scheil solidification simulation**. Click **Next**.



3. In the **Define Systems** window, choose an available **Database**.

4. Click to select **Elements** check boxes to include as system components. To add elements from an existing material file, click the **Material file** button to enter the file path to a material file or click the **Select Material File** button (to the right of the field) to navigate to a file on the computer.
5. Click **Next**.

The **Select Conditions** window has different options depending on the Project type and the elements selected.

In this example figure, using a **Single Point Equilibrium**, choose the **Composition unit** and under **Condition Definitions** specify the values of the state variables in the system.

For a **One axis equilibrium** or **Phase diagram**, specify the **Axis Definitions** of the stepping or mapping operation. Choose minimum and maximum values for the variable(s) (select **Linear – min no. of steps**, **Linear – max step size** or **Logarithmic – scale factors**) and whether it is **Normal** or **Separate phases**.

For a **Scheil solidification simulation**, and where applicable, select **Fast diffuser** to account for back diffusion of any fast-diffusing elements.

6. Click **Finish**.
7. Click to expand the **Event Log** window to see information about the progress of the calculation.

```

Event Log
12:12:02,234 INFO Global test at 5.20000E+02
12:12:02,249 INFO Terminating at 500.000
12:12:02,252 INFO *** Buffer saved on file: C:\Windows\TEMP\TH35C8~1\STATE_~1.POL
12:41:16,752 INFO Opened project file: Ex_05_Fe-C_stable_and_metastable_phase_diagram.tcu
12:42:17,239 INFO Opened project file: Ex_03_Fe-C_phase_diagram.tcu
14:11:35,181 INFO Define component C
14:11:35,181 INFO Define component Fe
14:11:35,211 INFO Performing general equilibrium calculation

```

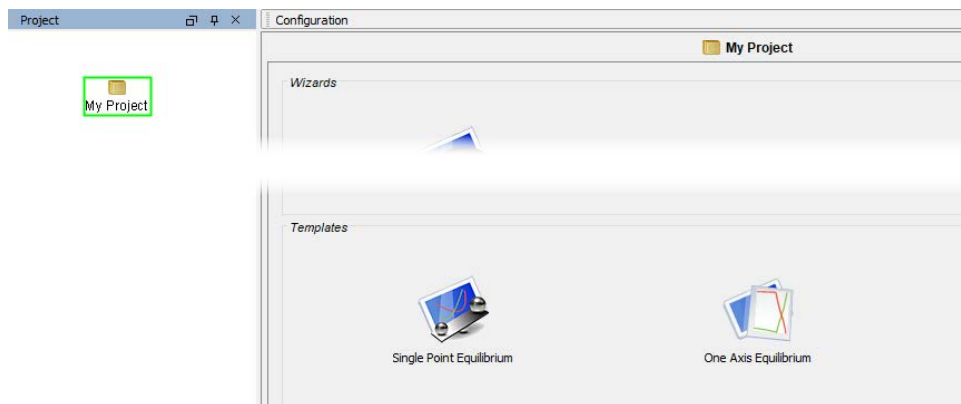
- The diagram is plotted in a **Plot Renderer** tab in the **Results** window. If you have calculated a single-point equilibrium, then a **Table Renderer** tab shows information about the equilibrium.

| Results | | | | |
|----------------------|----------------------|----------------------|------------------------|------------------|
| Table Renderer 1 | | | | |
| System | | | | |
| Moles | 1.00000 | | | |
| Mass | 12.01194 | [g] | | |
| Temperature | 1000.00000 | [K] | | |
| Total Gibbs Energy | -12659.53136 | [J] | | |
| Enthalpy | 11784.43824 | [J] | | |
| Volume | 5.39784E-6 | [m3] | | |
| <i>Component</i> | <i>Mole Fraction</i> | <i>Mass Fraction</i> | <i>Activity</i> | <i>Potential</i> |
| Fe | 0.00002 | 0.00010 | 0.00619 | -42278.5054 |
| C | 0.99998 | 0.99990 | 0.21816 | -12658.8942 |
| Stable Phases | | | | |
| | <i>Moles</i> | <i>Mass</i> | <i>Volume Fraction</i> | |
| BCC_A2#1 | 0.00002 | 0.00120 | 0.00003 | Composition |

- To save the project, click **Save** on the main toolbar. To save a diagram or table, right-click the diagram or table and select **Save As**.

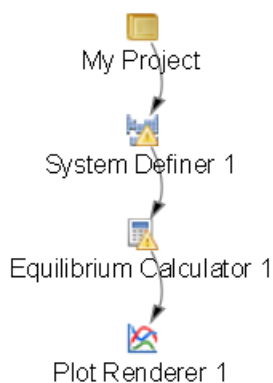
Creating a Project from a Template

Use a *Template* to create all the activities for a certain type of calculation. In the **Project** window click the **My Project** node to display the templates in the **Configuration** window.

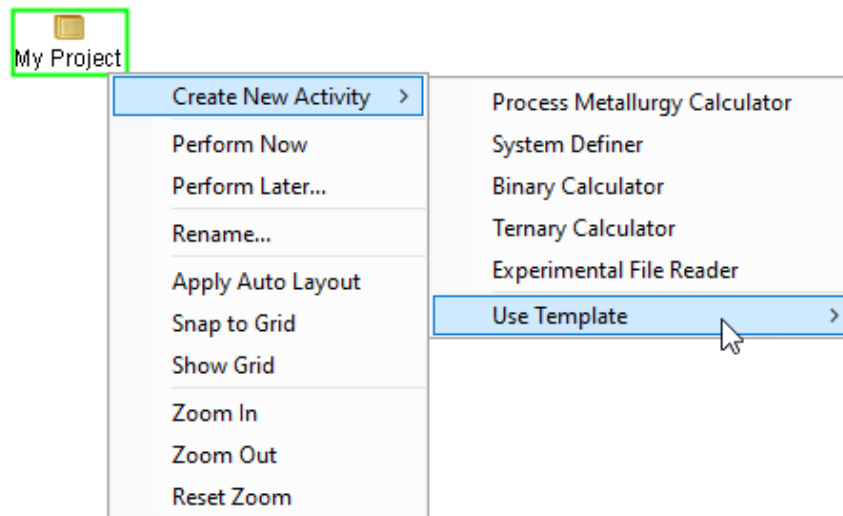


When you click a template, an activity tree is added to the **Project** window. You can then configure and perform the activities or the project.

For example, if you click **One axis equilibrium**, a tree is added to the **My Project** node with **System Definer**, **Equilibrium Calculator** and **Plot Renderer** nodes.



You can also add templates by right-clicking the **My Project** node and choosing an option from the **Create New Activity → Use Template** menu.



- ▶ ["The Quick Start Wizard and Templates" on page 26](#)
- ▶ ["Steel Library TTT Diagram Template" on the next page](#)

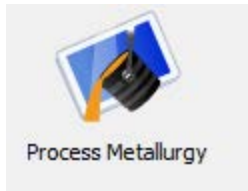
Process Metallurgy Template

Use a *Process Metallurgy* template to add the Process Metallurgy Calculator and a Plot Renderer to the **Project** window. The Process Metallurgy Calculator has several preconfigured settings making it easier to setup the different groups and materials needed to define a system for slag, metal and gas used in steelmaking.

- ▶ ["Process Metallurgy Calculator" on page 163](#)

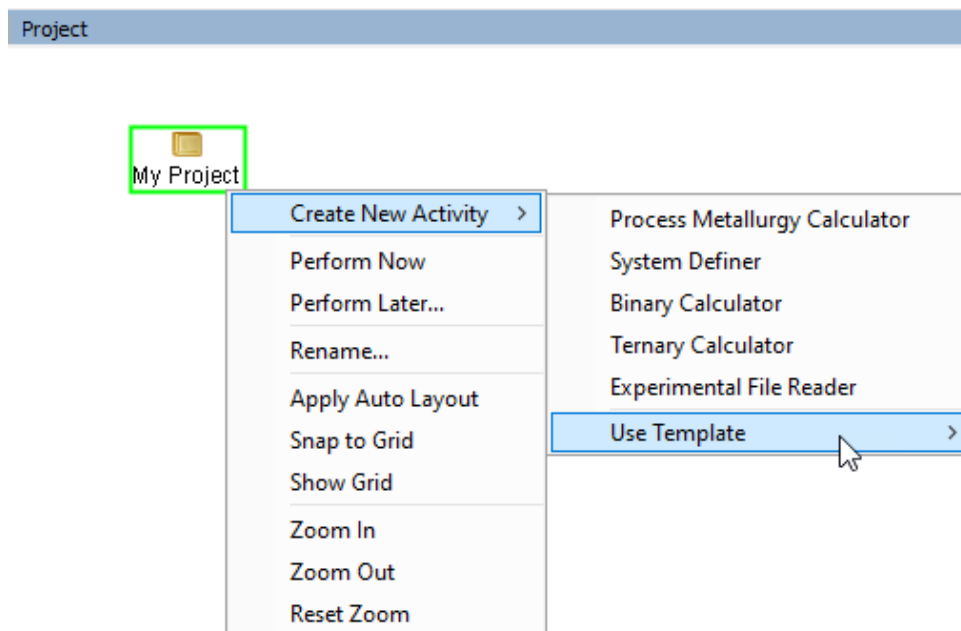
ADDING A PROCESS METALLURGY TEMPLATE TO A PROJECT

1. In the **Project** window click the **My Project** node to display the templates in the **Configuration** window.
2. Under *Templates*, click **Process Metallurgy**.



A **Process Metallurgy Calculator** and a **Plot Renderer** are added to the **Project** window.

You can also add templates by right-clicking the **My Project** node and choosing an option from the **Create New Activity → Use Template** menu.



Steel Library TTT Diagram Template



The use of this Steel Model Library template requires a valid maintenance license plus licenses for both the TCFE9 and MOBFE4 databases.

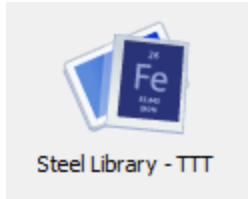
Use a *Steel Library TTT* template to add all the activities for a **One axis** Time-Temperature-Transformation (TTT) diagram calculation.

This template has several preconfigured settings to make it easy to set up and calculate the TTT diagram using the **Martensite temperatures** and **Pearlite** property models.

▶ ["Property Model Calculator" on page 75](#)

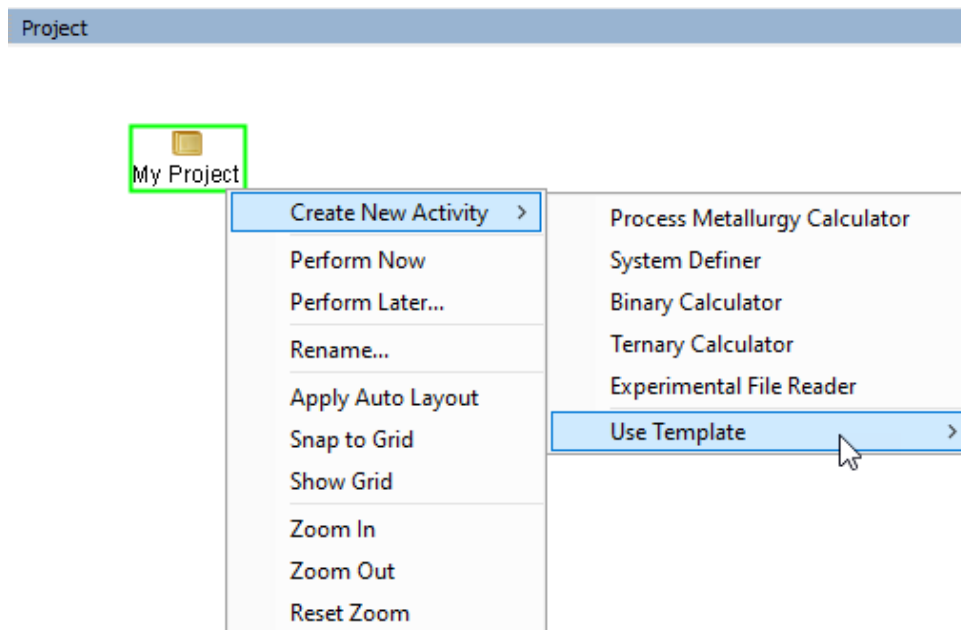
ADDING A STEEL LIBRARY TTT TEMPLATE TO A PROJECT

1. In the **Project** window click the **My Project** node to display the templates in the **Configuration** window.
2. Under *Templates*, click **Steel Library - TTT**.



A **System Definer**, *Property Model Calculator* (renamed to **Steel models**) and a *Plot Renderer* (renamed to **TTT**) are added to the **Project** window. Also see ["Plot Settings: TTT Mode" on page 185](#).

You can also add templates by right-clicking the **My Project** node and choosing an option from the **Create New Activity → Use Template** menu.



Defining and Using the Activity Nodes

In this section:

| | |
|-------------------------------------------|-----|
| System Definer | 36 |
| Equilibrium Calculator | 48 |
| Binary Calculator | 60 |
| Ternary Calculator | 63 |
| Scheil Calculator | 66 |
| Property Model Calculator | 75 |
| Diffusion Calculator | 109 |
| Precipitation Calculator | 129 |
| About the Process Metallurgy Module | 150 |
| Plot Renderer | 179 |
| Table Renderer | 194 |
| Experimental File Reader | 200 |

System Definer

In a System Definer activity, you select the database to use to retrieve thermodynamic data and define which elements the system has as components. You can also select the species to include as well as change the reference temperature and pressure for your components.

You can add the System Definer directly (right-click **My Project** and select it from the **Create New Activity** menu) or use a variety of the available templates to automatically add the node.



Almost all of the ["Graphical Mode Examples" on page 239](#) use the System Definer. For details about the templates, see ["The Quick Start Wizard and Templates" on page 26](#) and ["Creating a Project from a Template" on page 30](#).

Once you have added a System Definer, the **Configuration** window has these settings tabs:

- Elements
- Species
- Phases and Phase Constitution
- Components
- Data Sources
- Description

Define the System Definer Node


This topic describes how to define a system, specifically how to select one or more databases and define the elements in the system with the **System Definer** activity node.

1. Right-click **My Project** and from the menu select **Create New Activity→ System Definer** . You can also add any template and a System Definer is added to the Project tree.
2. In the **Project** window, click the **System Definer** activity node.
3. In the **Configuration** window, from the **Databases** menu choose **Database(s)** or a **Database Package**.



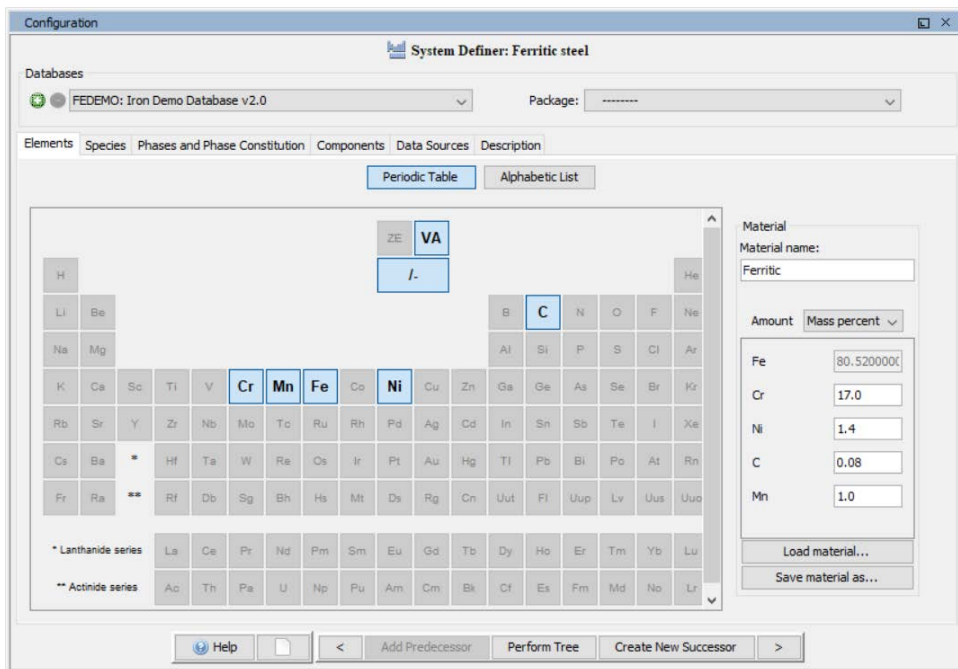
["About the Database Files" on page 31](#)

OPTIONS:

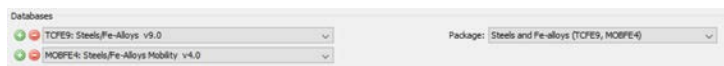
- Select **<User database>** to define your own.
 - You can choose to add one or more databases by clicking the **Add a database**  button.
 - From the **Package** list, choose a predefined database package to add multiple databases at a time. Depending on your license, there are predefined database packages available to select.
4. Select the **Elements** tab to choose the elements in the **Periodic Table** or use the **Alphabetic List** to choose elements for the system.
5. As required click the tabs to make edits: **Species**, **Phases and Phase Constitution**, and **Components**. The **Data Sources** and **Description** tabs provide information based on the database.
- ["Configuration Window Settings" below](#)
6. Click **Perform** to start the System Definer activity immediately and retrieve thermodynamic data about the system. Click the **Event Log** window to watch the progress of the job.


Configuration Window Settings

The **System Definer Configuration** window has many settings available, which are briefly described below.



CHOOSE DATABASE(S) OR A DATABASE PACKAGE



At the top of the **Configuration** window you can choose to add one or more databases by clicking the **Add a database**  button. You can also choose a predefined or custom database package from the **Package** list. Depending on your license, there are predefined database packages available to select.

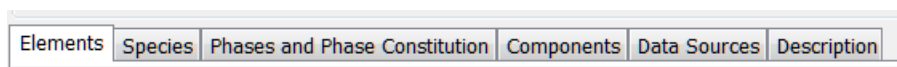
You can also click **Remove this database**  button as required.

► ["Global Settings: System Definer" on page 41](#)

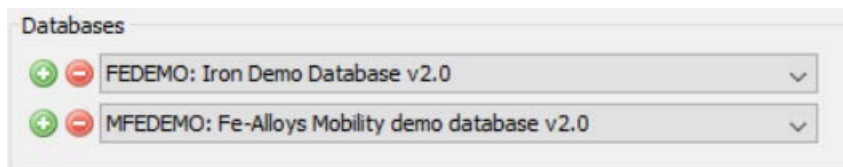


If you have chosen a database package and then remove or change a database, a message displays *Selected databases and selected package may differ*. This means that the original package you selected, which added preset databases, does not match the databases you are using for the project. For information about how to clear the message, see ["Global Settings: System Definer" on page 41](#).

There are several settings tabs available for the System Definer activity.



The following example uses the FEDEMO and MFEDEMO databases and Graphical Mode example PM_G_03.



ELEMENTS

On the **Elements** tab, and based on the databases or database package selected, you can select and review elements using a **Periodic Table** or **Alphabetic List** format. Unavailable elements are greyed out on the Periodic Table view.

PERIODIC TABLE

In this example, using the demonstration databases FEDEMO and MFEDEMO, there are only a select number of elements to choose from.

The periodic table shows the following elements highlighted in blue boxes:

- VA (Vanadium)
- I/- (Iodine)
- C (Carbon)
- Cr (Chromium)
- Mn (Manganese)
- Fe (Iron)
- Ni (Nickel)

ALPHABETIC LIST

| Element | FEDEMO | MFEDEMO |
|---------|-------------------------------------|-------------------------------------|
| I/- | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| C | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Cr | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Fe | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Mn | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Ni | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| VA | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |

MATERIAL COMPOSITION

On the **Periodic Table** page, you can also define the material composition:

Material

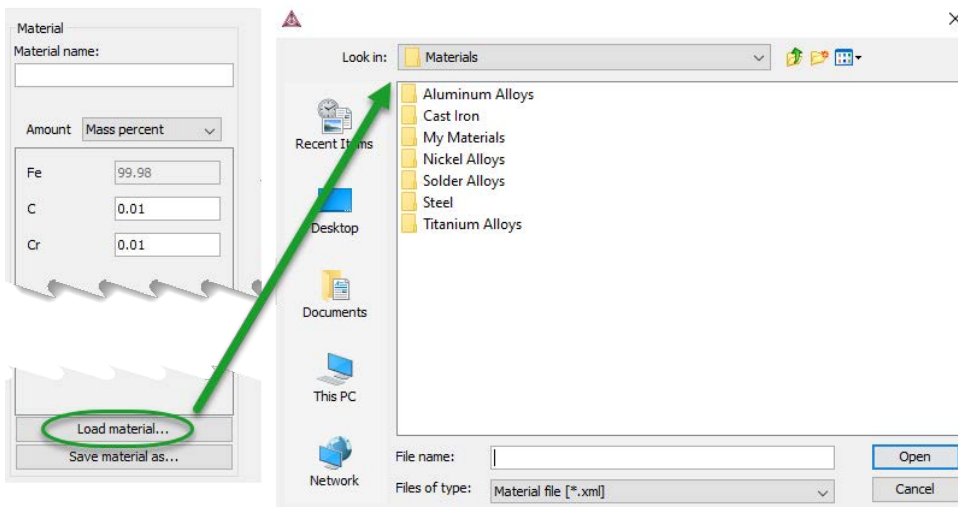
Material name:

Amount Mass percent ▾

| | |
|----|------------------------------------|
| Fe | <input type="text" value="80.52"/> |
| Ni | <input type="text" value="1.4"/> |
| C | <input type="text" value="0.08"/> |
| Mn | <input type="text" value="1.0"/> |
| Cr | <input type="text" value="17.0"/> |

At the bottom of the window, click **Load material** to open a material file. The default folder opens to the **Materials** folder included with your installation.

► ["About the Material Files" on page 44](#) and ["Examples, Manuals and Materials Folders" on page 17](#)



You can also click **Save material as** to save the material you defined, for example **Ferritic**.

► ["Global Settings: System Definer" on page 41](#)



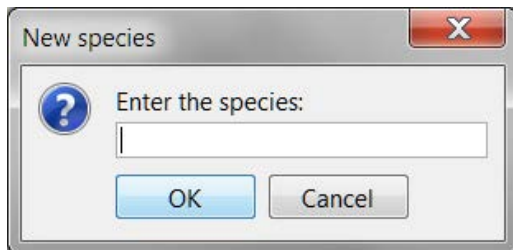
If you Load a material file and then change the composition, a message displays *The composition has changed*. This means that the original values/composition does not match the values you are using for the project. The message is cleared by either reloading the material file or editing the composition field to the original value.

SPECIES

On the **Species** tab for each database you can select and edit the **Species**.

| Elements | Species | Phases and Phase Constitution |
|----------|-----------------|-------------------------------------------------------------------------|
| Species | Stoichiometry | FEDEMO MFEDEMO |
| I. | -1 | <input checked="" type="checkbox"/> <input checked="" type="checkbox"/> |
| C | C | <input checked="" type="checkbox"/> <input checked="" type="checkbox"/> |
| Cr | Cr | <input checked="" type="checkbox"/> <input checked="" type="checkbox"/> |
| Fe | Fe | <input checked="" type="checkbox"/> <input checked="" type="checkbox"/> |
| Mn | Mn | <input checked="" type="checkbox"/> <input checked="" type="checkbox"/> |
| Ni | Ni | <input checked="" type="checkbox"/> <input checked="" type="checkbox"/> |
| VA | VA | <input checked="" type="checkbox"/> <input checked="" type="checkbox"/> |
| C2 | C ₂ | <input checked="" type="checkbox"/> <input type="checkbox"/> |
| C3 | C ₃ | <input checked="" type="checkbox"/> <input type="checkbox"/> |
| C4 | C ₄ | <input checked="" type="checkbox"/> <input type="checkbox"/> |
| C5 | C ₅ | <input checked="" type="checkbox"/> <input type="checkbox"/> |
| C60 | C ₆₀ | <input checked="" type="checkbox"/> <input type="checkbox"/> |

At the bottom of the window, click **Add new species** and enter the name of species in the field.



A dialog box titled "New species" with a close button (X) in the top right corner. Inside the dialog, there is a question mark icon and the text "Enter the species:". Below this text is a text input field. At the bottom of the dialog, there are two buttons: "OK" and "Cancel".

PHASES AND PHASE CONSTITUTION

| Status | Name | FEDEMO | MFEDMO |
|---------|-----------------|-------------------------------------|-------------------------------------|
| Entered | BCC_A2 | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Entered | CEMENTITE | <input checked="" type="checkbox"/> | <input type="checkbox"/> |
| Entered | CHI_A12 | <input checked="" type="checkbox"/> | <input type="checkbox"/> |
| Entered | DIAMOND_FCC_... | <input checked="" type="checkbox"/> | <input type="checkbox"/> |
| Entered | FCC_A1 | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Entered | FCC_A1#2 | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Entered | GAS | <input checked="" type="checkbox"/> | <input type="checkbox"/> |
| Entered | GRAPHITE | <input checked="" type="checkbox"/> | <input type="checkbox"/> |
| Entered | HCP_A3 | <input checked="" type="checkbox"/> | <input type="checkbox"/> |
| Entered | KSI_CARBIDE | <input checked="" type="checkbox"/> | <input type="checkbox"/> |
| Entered | LAVES_PHASE_... | <input checked="" type="checkbox"/> | <input type="checkbox"/> |
| Entered | LIQUID | <input checked="" type="checkbox"/> | <input type="checkbox"/> |
| Entered | M23C6 | <input checked="" type="checkbox"/> | <input type="checkbox"/> |
| Entered | M3C2 | <input checked="" type="checkbox"/> | <input type="checkbox"/> |
| Entered | M5C2 | <input checked="" type="checkbox"/> | <input type="checkbox"/> |
| Entered | M7C3 | <input checked="" type="checkbox"/> | <input type="checkbox"/> |
| Entered | SIGMA | <input checked="" type="checkbox"/> | <input type="checkbox"/> |

☒ Check/uncheck all

At the top of the **Phases and Phase Constitution** tab for each database, you can review and edit the **Status (Entered or Dormant)** for the selected **Phases**. Select the **Check/uncheck all** check box to toggle between the options.

To review the **Phase constitution** for a specific phase, click it in the **Phase** list (for example **BCC_A2**) and its details are displayed at the bottom of the window. Click **Edit** then click an element to select or reject a constituent. The last remaining constituent on a sublattice cannot be rejected.

FEDEMO

MFEDMO

Phase BCC_A2

Phase constitution for current system

Edit

(

Cr

Fe

Mn

Ni

)_{1.0}

(

C

VA

)_{3.0}

Phase description in database

(Cr,Fe,Mn,Ni)₁ (C,VA)₃

COMPONENTS

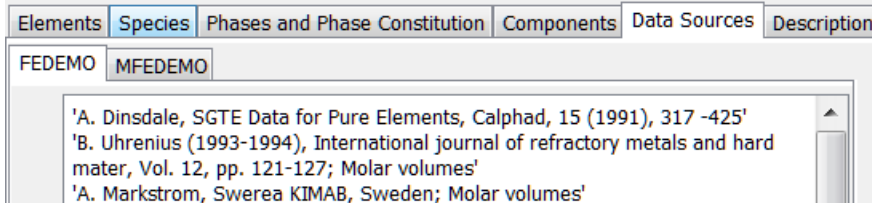
The **Components** tab is where you can review and edit the **Component, Reference phase,**

Reference temperature, and **Reference pressure**. Click to toggle the **SER** (Stable Element Reference) check box on and off. Then choose a **Reference phase** from the list and edit accordingly.

| Component | Reference phase | Reference temperature Kelvin | Reference pressure Pascal |
|-----------|------------------------------------------------|--------------------------------------------------------------|------------------------------|
| Fe | <input checked="" type="checkbox"/> SER HCP_A3 | <input checked="" type="checkbox"/> Current temperature 25.0 | 100000.0 |
| Cr | <input checked="" type="checkbox"/> SER | <input checked="" type="checkbox"/> Current temperature 25.0 | 100000.0 |
| Ni | <input checked="" type="checkbox"/> SER | <input checked="" type="checkbox"/> Current temperature 25.0 | 100000.0 |
| C | <input checked="" type="checkbox"/> SER | <input checked="" type="checkbox"/> Current temperature 25.0 | 100000.0 |
| Mn | <input checked="" type="checkbox"/> SER | <input checked="" type="checkbox"/> Current temperature 25.0 | 100000.0 |

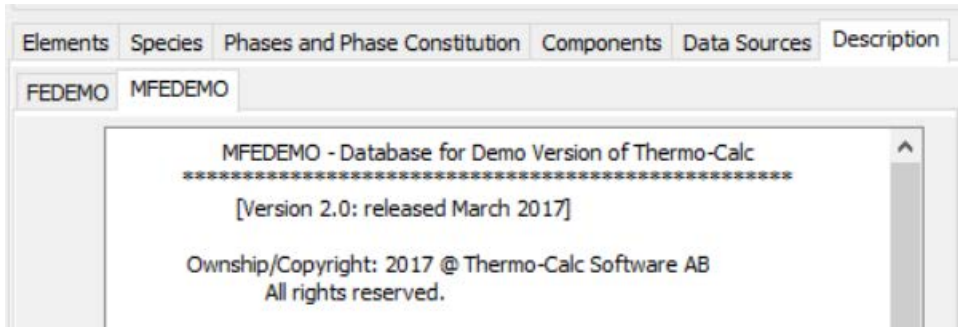
DATA SOURCES

Data sources are not available until the activity has been performed. Click **Perform Tree** to display available data sources.



DESCRIPTION

The **Description** tab displays a description of the selected database(s). In this example, **MFEDEMO**.



About the Material Files

► ["Examples, Manuals and Materials Folders" on page 17](#)

When you are working with the System Definer in Graphical Mode you can open the default **Materials** folder included with your installation. The files are in .xml format and the data contained are from some common alloys. You can also save and create your own materials files from the System Definer, or copy the xml files to the Materials folder.

ALUMINUM ALLOYS

- UNS_A95005
- UNS_A96053

CAST IRON ALLOYS

-
- UNS_F10007
 - UNS_F33101

NICKEL ALLOYS

- UNS_N06600
- UNS_N6600
- UNS_N06625
- UNS_N06690
- UNS_N07001
- UNS_N07718
- UNS_N08800
- UNS_N08825

SOLDER ALLOYS

- ASTM_25A
- ASTM_96TS
- UNS_L50134
- UNS_L54321

STEEL ALLOYS

Austenitic Stainless Steel

- ASTM_304_(UNS_S30400)
- ASTM_304L_(UNS_S30403)
- ASTM_304LN_(UNS_S30453)
- ASTM_316_(UNS_S31600)
- ASTM_316L_(UNS_S31603)
- ASTM_316LN_(UNS_S31653)
- ASTM_317L_(UNS_S31703)

-
- UNS_J92710
 - UNS_S30908

Duplex Stainless Steel

- UNS_S31803_A
- UNS_S32750_A
- UNS_S32750_B

High Speed Steel

- ASTM_M10_A5

High Temperature Steel

- UNS_S31008

HSLA Steel

- UNS_K12000

Low Carbon Steel

- UNS_H61180

Maraging Steel

- UNS_K92810

Martensitic Stainless Steel

- ASTM_420
- UNS_J82090
- UNS_J91639
- UNS_S44004

Tool Steel

- UNS_T30106
- UNS_T30109

-
- UNS_T51620

Training Steel

- Ferritic
- M7_Steel

TITANIUM ALLOYS

- UNS_R54520
- UNS_R56260

My MATERIALS

This is where you can add your own material files to be able to load it to the System Definer. When you are in the System Definer Configuration window, you define your material then click **Save material as**. You can save the profile to this folder or create a folder with a new name.

Equilibrium Calculator

An Equilibrium Calculator allows you to set the conditions for, and perform, a calculation. You can add the calculator to the System Definer directly (right-click and select it from the **Create New Successor** menu) or use a variety of the available templates.

Once you have added an Equilibrium Calculator, the **Configuration** window has these settings tabs. An Equilibrium Calculator that is the successor of another Equilibrium Calculator inherits all the Configuration window settings of the predecessor.

- **Conditions:** Set the conditions for your calculation that define the stepping or mapping axis variables. This tab can be viewed in a simplified mode and in an advanced mode.
- **Functions:** Define your own quantities and functions, which you then can calculate and plot.
- **Options:** Modify numerical settings that determine how equilibria are calculated, as well as how stepping and mapping calculations are performed.



The **Options** tab is where you can locally define specific Equilibrium Calculator settings. These settings can also be applied globally. To open the Options window: From the main menu select **Tools → Options** and click the **Activities** tab. Then click **Calculation**.



For an example of how serially coupled Equilibrium Calculators can be used, see [example T_06](#). For details about the templates, see "[The Quick Start Wizard and Templates](#)" on page 26 and "[Creating a Project from a Template](#)" on page 30.

Define the Equilibrium Calculator

1. Add an **Equilibrium Calculator** node to the System Definer. If you used the **Single Point Equilibrium**, **One-Axis Equilibrium**, or **Phase Diagram** template, click the Equilibrium Calculator node to display the **Configuration** settings window.
2. In the **Configuration** window, enter the settings described in "[Conditions Tab Settings](#)" on the next page, and as required from the "[Options Tab Settings](#)" on page 53. There are also settings you can define on the **Functions** tab. See "[Calculating and Plotting Functions](#)" on page 51
3. Once you have finished defining the Equilibrium Calculator, you also choose settings on the "[Plot Renderer](#)" on page 179.



["Calculating with a Fixed Phase " on page 57](#)

Conditions Tab Settings

Conditions and axis variables for the Equilibrium Calculator are set in the **Conditions** tab of the Configuration window. The tab can be viewed in two modes: **simplified** (the default) or **advanced**. The conditions to set depend on the type of calculation.

The screenshot shows the 'Conditions' tab of the Equilibrium Calculator configuration window. It has three sub-tabs: 'Conditions', 'Functions', and 'Options'. The 'Composition unit' is set to 'Mass percent'. Under 'Condition Definitions', 'Temperature' is set to 'Celsius' at 1000.0, 'Pressure' is set to 'Pascal' at 100000.0, and 'System size' is set to 'Mole' at 1.0. Under 'Calculation Type', 'Phase diagram' is selected with a radio button. Under 'Axis Definitions', there are two rows, both for 'Temperature', with 'Min' at 500.0, 'Max' at 3000.0, 'Step division' at 50.0, and 'Type' set to 'Linear - min no. of steps'.



See examples ["T_01: Calculating a Single-Point Equilibrium" on page 240](#) , ["T_02: Stepping in Temperature in the Fe-C System" on page 242](#) and ["T_05: Stable and the Metastable Fe-C Phase Diagrams" on page 249](#).



["Options Tab Settings" on page 53](#)

ABOUT ADVANCED MODE

Click **Switch to advanced mode** to add and remove conditions as well as set additional axis definitions. However, the number and types of conditions set must still conform to the Gibbs' phase rule. The **Number of missing conditions is** field, at the top of the tab shows how many conditions that you have left to set. If the number is negative, then that number of conditions need to be removed.

The following outlines what you can set on the **Conditions** tab in simplified mode.



Click **Switch to advanced mode** for more options.

Composition unit

Choose from **Mass percent**, **Mole percent**, **Mass fraction** or **Mole fraction**.

Condition Definitions

Specify the values (and units) of the state variables: **Temperature**, **Pressure**, and **System size**.

Calculation Type

Single equilibrium (no axes), **One axis**, **Grid** or **Phase diagram**.



Single equilibrium only calculates the equilibrium. No additional settings are required. Add a **Table Renderer** to perform the calculation and view the details in the **Results** window.



When you use the ["Equilibrium Model" on page 80](#) with the **Property Model Calculator**, it is the same calculation result as when you are using an **Equilibrium Calculator** with the **Single equilibrium** calculation type.

Axis Definitions

- **One axis**: Define the axis variable using these fields and menus: **Quantity**, **Min**, **Max**, **Step division** and **Type**.
- **Grid**: Define the two axis variables using these fields and menus: **Quantity**, **Min**, **Max** and **Number of steps**.
- **Phase diagram**: Define the two axis variables using these fields and menus: **Quantity**, **Min**, **Max**, **Step division** and **Type**.



If the Equilibrium Calculator already has a Plot Renderer as a successor and you change the stepping/mapping quantities, then the quantities represented on the X- and Y-axis are automatically updated in the Plot Renderer.



For a **One axis**, on the Plot Renderer, you can choose to plot a *Heat map*, *Contour* or *3D diagram*.

Number of steps (Grid)

Set a fixed **Number of steps**. The number of steps along with the minimum and maximum values for the axes define a grid. For each grid point an equilibrium is calculated.

Type and Step division (One axis and Phase diagram)

Type options: **Linear - min no. of steps**, **Linear - max step size** and **Logarithmic - scale factor**.


- For *Linear - min no. of steps*, the **Step division** value specifies a minimum number of steps that is calculated between the minimum and maximum value during the stepping/mapping operation.
- For *Linear - max step size*, the **Step division** sets the maximum size of each step. For *Logarithmic - scale factor*, **Step division** specifies the scale factor of a logarithmic function that distributes the steps from the initial equilibrium to the minimum and maximum values defined.

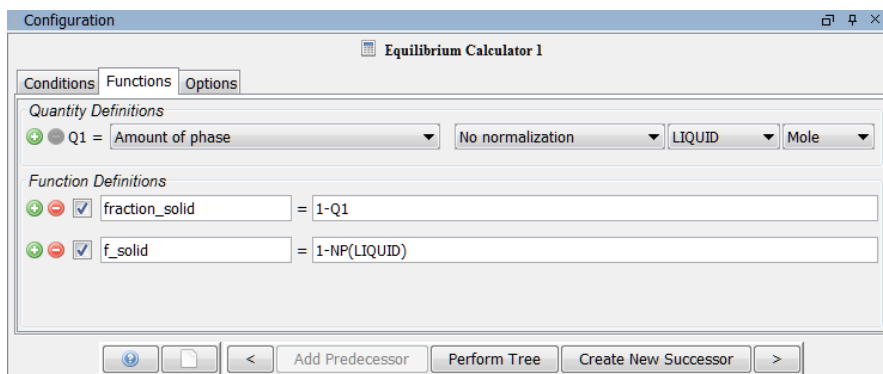
Calculating and Plotting Functions


The **Functions** tab allows you to define your own functions that can be plotted in a Plot Renderer.



For an example of how you can use functions that you define, see ["T_07: User-Defined Functions" on page 256](#).

1. Add an **Equilibrium Calculator** node and click it in the **Project** window.
2. In the **Configuration** window click the **Functions** tab.
3. Under **Quantity Definitions**, define **Q1**. Click the add  button to **Add a new quantity**. Then from the lists, choose the variable for each quantity to define. The quantities are called **Q1**, **Q2**, **Q3** and so on. In this example, the quantity **Q1** is defined as the **Amount of phase**, with **No normalization**, **LIQUID** in **Mole** units.



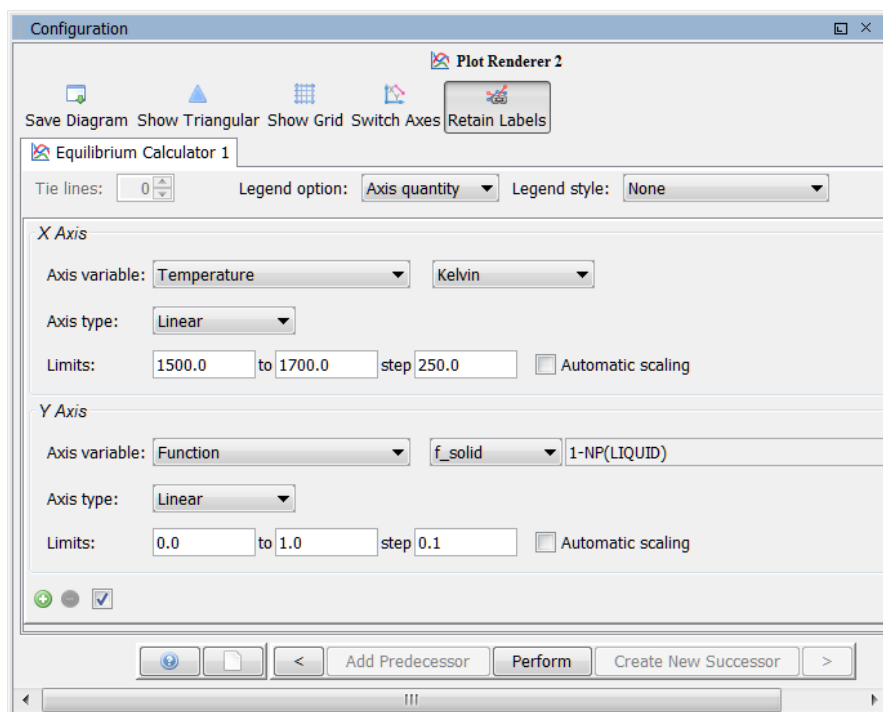
4. Under **Function Definitions**, click the add  button to add a new function. In the left field edit the default name of each function and enter the function itself in the right field after the equal sign. In this example, the quantity defined as Q1 is renamed to **fraction_solid**, which gives as its output the fraction of solid phase (**1-Q1**).



You can also use Console Mode syntax when entering the function. For example, the function above can be entered as `1-NP(LIQUID)`. See ["Parameters, Functions and Variables" on page 378](#) for details related to Console Mode and that are also applicable here.

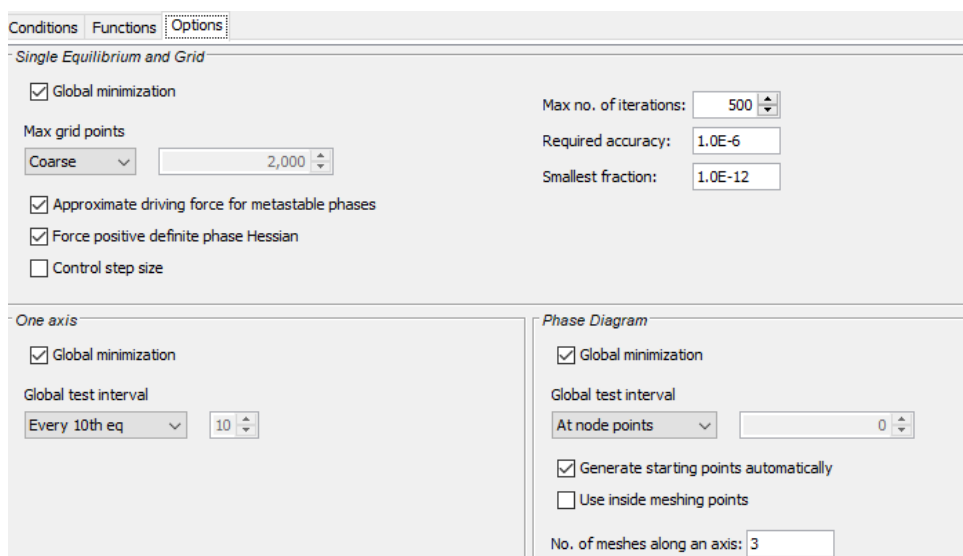
5. To plot the defined function, right-click **Equilibrium Calculator** and choose **Create new successor**→**Plot Renderer**.
6. Click the **Plot Renderer** node. In the tab for the Equilibrium Calculator that contains the function, set an **Axis variable** to **Function**, then from the menu select the defined function. In this example the Y-axis is set to plot the value of the function **fraction_solid**.

When run, the Plot Renderer plots the value of the function.



Options Tab Settings

These settings are for the ["Equilibrium Calculator" on page 48](#) and are located on the **Configuration** window → **Options** tab.





You can change these settings locally for a specific Equilibrium Calculator or globally in the **Options** settings. To open the Options window: From the main menu select **Tools** → **Options**. Click the **Graphical Mode** tab then click **Calculation**.

Single Equilibrium and Grid

Global minimization

The check box is selected by default to ensure that the most stable minimum under the specified conditions is computed.

Max grid points

Coarse (2000 grid points, the default), **Medium** (20,000 grid points), **Fine** (200,000 grid points), or **Custom** (set your own number of grid points).

Approximate driving force for metastable phases

The check box is selected by default, which means the metastable phases are included in all iterations. However, these may not have reached their most favourable composition and thus their driving forces may be only approximate.

If it is important that these driving forces are correct, click to clear the check box to force the calculation to converge for the metastable phases.

Force positive definite phase Hessian

The check box is selected by default and this setting determines how to reach the minimum of an equilibrium state.

▶ ["ADVANCED_OPTIONS" on page 135](#)

Control stepsize

The check box is selected by default and this setting determines how to reach the minimum of an equilibrium state.

▶ ["ADVANCED_OPTIONS" on page 135](#)

Max no of iterations

By default, the program tries 500 iterations before it gives up. As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.

Required accuracy

The default is 1.0E-6. This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.

Smallest fraction

The default is 1.0E-12. This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions.

The default value for the smallest site-fractions is 1E-12 for all phases except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as 1E-30.



In Console Mode, the default of 1E-30 for IDEAL phases is true unless you are using the command SET_NUMERICAL_LIMITS to reset an even-lower value (e.g. 1E-45, that is naturally enforced to all the phases in the system).

One Axis

Global minimization

The check box is selected by default to ensure that the most stable minimum under the specified conditions is computed.

▶ ["ADVANCED_OPTIONS" on page 135](#)

Global test interval

Every 10th eq (the default), **Always** or **Custom**.

The default is the recommended global test interval i.e. every tenth step and at each phase change during calculations.

If you choose **Custom**, the integer number determines how often the Global Minimization should be used during step and mapping. Any other positive integer number, n , suggests it performs a Global Minimization test at every n -th step during calculations.

Phase Diagram

Global minimization

The check box is selected by default to ensure that the most stable minimum under the specified conditions is computed.

Global test interval

At node points (the default), **Every 10th eq**, **Always** or **Custom**.

The default is the recommended global test interval is used only at node points during the calculations.

If you choose **Every 10th eq**, this is every tenth step and at each phase change during calculations.

If you choose **Custom**, the integer number determines how often the Global Minimization should be used during step and mapping. Any other positive integer number, n , suggests it performs a Global Minimization test at every n -th step during calculations.

Generate starting points automatically

The check box is selected by default.

Use inside meshing points

Click to select the check box as required. The initial mesh consists of initial equilibrium points added only along the edge/border of the diagram defined by the axis-variables. If you select the check box, then the initial equilibrium points added are also added to the inside edge.

No of meshes along an axis

The default is 3, which represents how many intervals of initial equilibrium points are added along an edge in the diagram. For example, if set to 2 (two), initial equilibrium points are added at the beginning, center, and end of each axis-variable forming 2 intervals.

Calculating with a Fixed Phase

This describes how to use the advanced mode to set a phase to be fixed at a certain amount. This allows you to, for example, find out at what temperature a material starts to melt. If you set the phase to be fixed to liquid phase at zero amount, and do not define the temperature state variable, then you can calculate at what temperature the material enters a state where the liquid phase is no longer zero (that is, when it starts to melt).



For a fixed phase equilibrium calculation, it is recommended to serially couple the Equilibrium Calculators. This is where one Equilibrium Calculator activity is the successor to another Equilibrium Calculator activity that performs an ordinary equilibrium calculation, and then, for the condition you are interested in, you make a rough estimate of the value. This gives the fixed phase calculation better starting values.

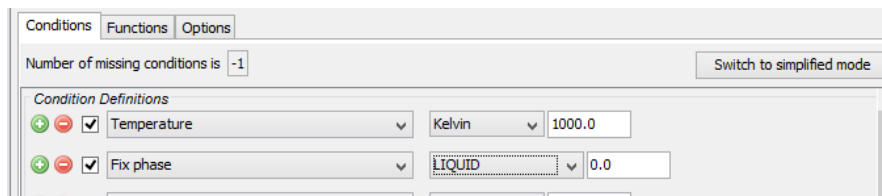
1. Right-click a node that can add an **Equilibrium Calculator** to your project.
2. In the **Project** window, click the **Equilibrium Calculator** activity node.
3. In the **Configuration** window, click **Switch to advanced mode**.



If the **Default calculation mode** is globally set to **Advanced** then by default the Configuration window is already in advanced mode.

▶ ["Changing Global Settings" on page 36](#)

4. Under **Condition Definitions**, click the **Add quantity** button.
5. Select **Fix phase** from the first menu.
6. Select the phase that you want to fix in the second menu, and set the amount of that phase you want to fix the phase to. For example, if you want to know when your material starts to melt, set the phase to **LIQUID** and the value to **0.0**:



Above the condition definitions, the **Number of missing conditions is** field is probably **-1**. This means that you must remove one condition.

7. To remove a condition, either click the remove button, or click to clear the checkbox. For example, if you want to know at what temperature your material starts to melt, then you cannot have a fixed temperature, in which case the temperature condition is not selected:

The screenshot shows a software interface with three tabs: 'Conditions', 'Functions', and 'Options'. The 'Conditions' tab is active. At the top, it says 'Number of missing conditions is 0' next to a small input box containing '0'. To the right of this is a button labeled 'Switch to simplified mode'. Below this is a section titled 'Condition Definitions'. It contains two rows of settings. The first row has a green plus icon, a red minus icon, an unchecked checkbox, the text 'Temperature', a dropdown menu showing 'Kelvin', and a text box with '1000.0'. The second row has a green plus icon, a red minus icon, a checked checkbox, the text 'Fix phase', a dropdown menu showing 'LIQUID', and a text box with '0.0'. There is a vertical scrollbar on the right side of the 'Condition Definitions' section.

The **Number of missing conditions** field displays **0**. When you have set all your conditions, you can perform the Equilibrium Calculator (now or later).

Binary Calculator

A Binary Calculator can be used for some calculations involving two components. You can think of this activity as a combination of a System Definer and an Equilibrium Calculator, but designed to simplify setting up and performing calculations on binary systems. There is also a **Binary Calculation** template you can use to quickly set up a simulation.

The Binary Calculator relies on some specifications that are not supported by all databases. You need a specially designed database for the Binary Calculator such as the TCBIN database.



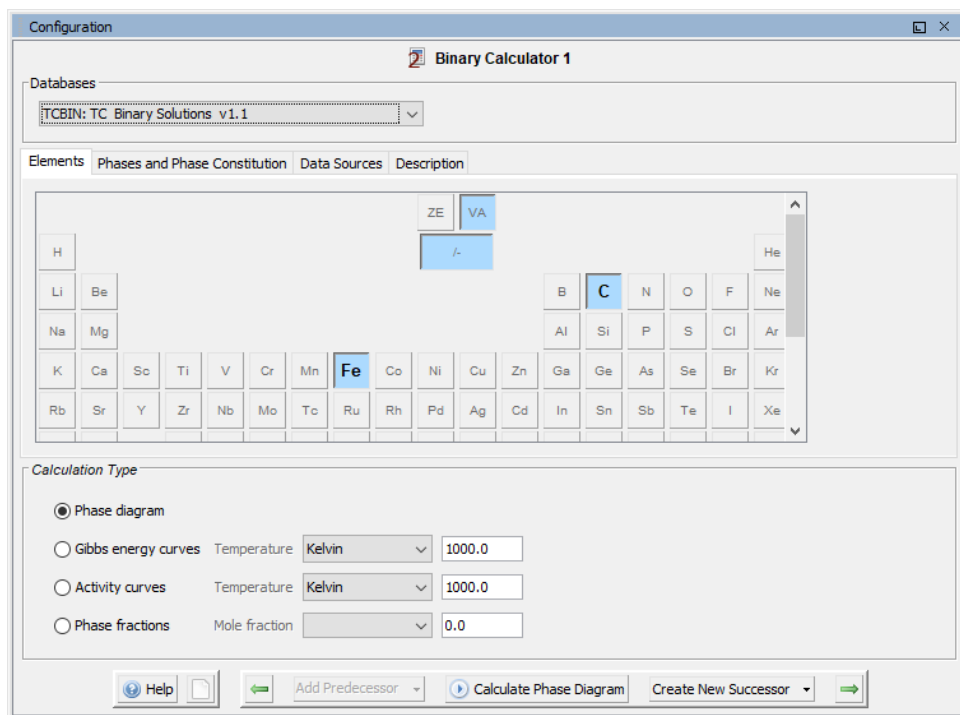
For an example of how a Binary Calculator can be used in a project, see ["T_03: Fe-C Phase Diagrams" on page 244](#). For information about the templates see ["Creating a Project from a Template" on page 30](#).

Configuration Window Settings

The **Binary Calculator Configuration** settings window and the associated tabs are similar to what you see on a System Definer. The database TCBIN is added by default when you use the Binary Calculation template, but you can choose any installed and licensed database from the list.



The various versions of the TCFE (Thermo-Calc Steels and Fe-Alloys) databases are not compatible with the Binary Calculator.



Elements

On the **Elements** tab, and based on the database selected, select and review elements using a **Periodic Table** format. Unavailable elements are greyed out on the Periodic Table view.

Phases and Phase Constitution

At the top of the **Phases and Phase Constitution** tab, and based on the selected database, you can review the **Status** for the selected **Phases**. Select the **Check/uncheck all** check box to toggle between the options.

To review the **Phase constitution** for a specific phase, click it in the **Phase** list (for example **BCC_A2**) and its details are displayed at the bottom of the window. Click **Edit** then click an element to select or reject a constituent. The last remaining constituent on a sublattice cannot be rejected.

Data Sources

Data sources are not available until the activity has been performed. Click **Perform Tree** to display available data sources.

Description

The **Description** tab displays a description of the selected database.

Calculation Type

Choose a calculation type.

Phase diagram

Select to perform a mapping calculation. Click **Calculate Phase Diagram** to plot the results.

Gibbs energy curves

Select the **Temperature** and click **Calculate Gibbs Energy Curves** to calculate at a constant temperature over the whole composition range.

Activity curves

Select the **Temperature** and click **Calculate Activity Curves** to calculate at a constant temperature over the whole composition range.

Phase fractions

Select the **Mole fraction** and click **Calculate Phase Fractions** to calculate as a function of temperature at a constant composition.

Ternary Calculator

A Ternary Calculator is used for some calculations involving three components. You can think of this activity as a combination of a System Definer and an Equilibrium Calculator, but designed to simplify setting up and performing calculations on ternary systems. There is also a **Ternary Calculation** template you can use to quickly set up a simulation.



For an example of how a Ternary Calculator is used in a project, see ["T_04: Fe-Cr-C Ternary Phase Diagram at 1000 K" on page 246](#). For information about the templates see ["Creating a Project from a Template" on page 30](#).

Configuration Window Settings

Below lists the available settings that must be configured before performing the calculation and the image shows the Configuration window of a Ternary Calculator activity.

Configuration

Ternary Calculator 1

Databases
TCFE8

Elements Phases and Phase Constitution Data Sources Description

Periodic table elements: H, He, Li, Be, Na, Mg, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Br, Kr, Rb, Sr, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, Te, I, Xe, Cs, Ba, * Hf, Ta, W, Re, Os, Ir, Pt, Au, Hg, Tl, Pb, Bi, Po, At, Rn, Fr, Ra, ** Rf, Db, Sg, Bh, Hs, Mt, Ds, Rg, Cn, Uut, Fl, Uup, Lv, Uus, Uuo.

* Lanthanide series: La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu
** Actinide series: Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr

Calculation Type

☒ Isothermal section Temperature Kelvin 1000.0

☐ Monovariant lines

☐ Liquidus projection Temperature Kelvin Min 298.15 Max 3273.15 Interval 100.0

Buttons: Add Predecessor, Perform Tree, Create New Successor, navigation arrows.

Databases

Select a database that contains specifications dedicated to the Ternary Calculator.

Elements

On the **Elements** tab, and based on the database selected, select and review elements using a **Periodic Table** format. Unavailable elements are greyed out on the Periodic Table view.

Phases and Phase Constitution

At the top of the **Phases and Phase Constitution** tab, and based on the selected database, you can review the **Status** for the selected **Phases**. Select the **Check/uncheck all** check box to toggle between the options.

To review the **Phase constitution** for a specific phase, click it in the **Phase** list (for example **BCC_A2**) and its details are displayed at the bottom of the window. Click **Edit** then click an element to select or reject a constituent. The last remaining constituent on a sublattice cannot be rejected.

Data Sources

Data sources are not available until the activity has been performed. Click **Perform Tree** to display available data sources.

Description

The **Description** tab displays a description of the selected database.

Calculation Type

Choose a calculation type.

Isothermal section

Select the **Temperature** at which the ternary system is calculated for the whole composition range.

Monovariant lines

To calculate the variation of the liquid compositions with temperature.

Liquidus projection

Select the **Temperature** range (**Min** and **Max**) and an **Interval**. The projection liquid surface and the monovariant lines are calculated over the given temperature range.

Scheil Calculator

Thermo-Calc is often used to perform equilibrium calculations, but some non-equilibrium transformations or partial-equilibrium transformations can also be simulated.

A well known example of a non-equilibrium calculation is the *Scheil-Gulliver solidification simulation*.

Classic Scheil Simulation

For the *Scheil-Gulliver solidification simulation*, generally referred to in Thermo-Calc as a classic *Scheil simulation*, the following assumptions are made.

- Diffusion in the liquid phase is assumed to be very fast, that is, infinitely fast.
- Diffusion in the solid phases is so slow that it can be ignored, that is, diffusion is assumed to be zero.
- The liquid/solid interface is in thermodynamic equilibrium.

In this Scheil simulation the temperature is decreased step-by-step. When the temperature drops below the liquidus temperature the equilibrium amount and composition of solid and liquid phase is calculated. The solid phase is removed from the system and only the amount and composition of the liquid phase is used for the next calculation step at a lower temperature. Again, the equilibrium amount and composition of solid and liquid phase is calculated and again the solid phase is removed from the system for the next step. This procedure is repeated until the last liquid disappears.

This calculation procedure is equivalent to assuming that there is no diffusion in the solid phase and infinitely fast diffusion of all elements in the liquid phase. It has been shown to be a good approximation of the solidification of most alloys such as Ni-superalloys, Cu alloys, Al alloys, Mg alloys, and others. However, for steels it fails badly. The reason is that carbon is one of the most important alloying elements in steels and it dissolves interstitially. Carbon therefore has very fast diffusion rates. The assumption of no diffusion in the solid phase during solidification is thus not correct for carbon at most industrial or lab-scale solidification rates.

For this reason a variant of the Scheil simulation was developed and implemented in Thermo-Calc, where one or more elements can be defined as *fast diffusers*.

Scheil Simulation with a Fast Diffuser Element

The *Scheil simulation with fast diffuser* model in Thermo-Calc takes into account the concept of the *fast diffuser*. Typically, C is defined as a fast diffuser, but also other elements such as N, O, or others can also be defined.



Fast diffuser does not quite define this since diffusion is not actually simulated. It is simply assumed that the “fast diffusers” distribute throughout the solid and liquid phase according to thermodynamic equilibrium. This corresponds to *infinitely fast diffusion*.

For the *Scheil simulation with fast diffuser* the following assumptions are made.

- Diffusion of all elements in the liquid phase is infinitely fast.
- Diffusion of all elements in the solid phases, except the ones defined as “fast diffusers”, is zero.
- Diffusion of the elements defined as “fast diffusers” is infinitely fast in the solid phase.
- The liquid/solid interface is in thermodynamic equilibrium.

The classic Scheil simulation and Scheil simulation with fast diffuser models can be considered *thermodynamic* models. There are clear limitations as a certain amount of back diffusion always takes place in the solid phase at real solidification. For this reason, a more sophisticated kinetic model, the *Scheil simulation with back diffusion* is also available.

Scheil Simulation with Back Diffusion

The *Scheil simulation with back diffusion* kinetic model quantitatively takes into account the real back diffusion of all elements in the primary solid phase (typically the FCC or BCC phase). This model requires the use of both a thermodynamic and mobility database. The calculation also requires the cooling rate to be specified; a fast cooling rate allows for less time for back diffusion and the simulation result is similar to the classic Scheil-Gulliver solidification simulation. A very slow cooling rate allows for almost complete back diffusion, the solidification simulation is then close to an equilibrium calculation. It also requires that the size of the solidification domain is specified. In most cases this domain size corresponds to the secondary arm spacing, as this is where typically the liquid is trapped during solidification.



The secondary arm spacing also depends on the cooling rate. For this reason a simple empirical relation between cooling rate and secondary arm spacing is predefined in Thermo-Calc.

For the Scheil simulation with back diffusion the following assumptions are made.

-
- Diffusion of all elements in the liquid phase is infinitely fast.
 - Diffusion of all elements in the primary solid phase are quantitatively calculated using mobility data, a cooling rate and a domain size (typically this is the secondary arm spacing).
 - The liquid/solid interface is in thermodynamic equilibrium.

Summary

The variants of the Scheil-Gulliver solidification simulation (classic Scheil simulation, Scheil with a fast diffuser element, and Scheil with back diffusion) are set up in either the SCHEIL module in Console Mode or the Scheil Calculator in Graphical Mode.



The Scheil with back diffusion feature is only available for systems with diffusion data, i.e. it requires the use of a mobility database.

The Scheil calculation allows the calculation of:

- The solidification range of an alloy.
- Depression of the solidus temperature due to segregation.
- Composition of the last liquid to disappear in segregation pockets.
- Phases formed on final solidification in segregation pockets.
- The composition gradient in the primary solid phase(s) (segregation profile).

By default, a Plot Renderer successor to a Scheil Calculator has the default plot axes **Mole fraction of solid** (X-axis) and **Temperature Celsius** (Y-axis). When these default axes are used in the Plot Renderer, the results of normal equilibria calculations are automatically plotted in the same diagram as the Scheil calculations.

You can use either the **Quick Start Wizard** (for only Scheil-Gulliver) or the **Scheil Solidification Simulation** template to quickly set up a simulation.



For information about the templates see ["Creating a Project with the Quick Start Wizard" on page 28](#) and ["Creating a Project from a Template" on page 30](#).



For examples using the Scheil Calculator see ["T_08: Scheil and Equilibrium Solidification" on page 258](#) and ["T_10: Scheil Solidification with Back Diffusion" on page 263](#).

Define the Scheil Calculator

1. Add a **Scheil Calculator** node to the System Definer. If you used the **Scheil Solidification Simulation** template, click the node to display the **Configuration** settings window.
2. Enter the settings described in ["Configuration Window Settings" below](#). This includes details about the Advanced Options settings.
3. Once you have finished defining the Scheil Calculator, you also choose settings on the ["Plot Renderer" on page 179](#).

Configuration Window Settings

An example of the main **Configuration** window of a **Scheil Calculator** activity is shown below. These settings must be configured before performing the calculation.

The screenshot shows the 'Configuration' window for 'Scheil Calculator 1'. The window has a title bar with 'Configuration' and standard window controls. Inside, there's a section for 'Scheil Calculator 1' with a 'Show advanced options' button. The settings are as follows:

| Parameter | Value | Unit/Option |
|----------------------------------|--------------------------|-------------|
| Start temperature: | 2500.0 | |
| Temperature step: | 1.0 | |
| Temperature unit: | Kelvin | Dropdown |
| Composition unit: | Mole percent | Dropdown |
| Back diffusion in primary phase: | <input type="checkbox"/> | |

| Composition | Value | Fast diffuser |
|-------------|-------|--------------------------|
| Al | 96.9 | <input type="checkbox"/> |
| Cu | 2.1 | <input type="checkbox"/> |
| Si | 1.0 | <input type="checkbox"/> |

At the bottom, there's a toolbar with buttons: Help, Add Predecessor, Perform, and Create New Successor.

Start temperature

Enter a **Start temperature** that is higher than the liquidus temperature of the alloy, in other words, the temperature at which the alloy is completely melted.

Temperature step

Enter a **Temperature step**. Decreasing the temperature step increases the accuracy, but the

default value is usually adequate.

Temperature unit

Select the **Temperature unit**: Kelvin, Celsius or Fahrenheit.

Composition unit

Select the **Composition unit**: Mass percent, Mole percent, Mass fraction or Mole fraction.

Back diffusion in primary phase



The Scheil with back diffusion feature is only available for systems with diffusion data, i.e. it requires the use of a mobility database.

The **Back diffusion in primary phase** check box is available to select after adding a mobility database and once components are defined on the System Definer. Click to select this check box to enable back diffusion in the solid primary phase.



See "[Scheil Calculator](#)" on page 66 for an overview of the different Scheil simulation models available and more information about this model.

Cooling rate (available with back diffusion)

This field is available when the **Back diffusion in primary phase** check box is selected.

Specify the **Cooling rate** in Kelvin per second (K/s). An increased value moves the result from equilibrium toward a Scheil-Gulliver calculation.

Secondary dendrite arm spacing (available with back diffusion)

This field is available when the **Back diffusion in primary phase** check box is selected.

The **Secondary dendrite arm spacing** is the distance in meters between two secondary dendrite arms. It can be either a **Constant** or **Calculated** from the cooling rate as $c \cdot (\text{cooling rate})^{-n}$ where c and n are entered in these fields.

Select **Calculated** or **Constant**.

- For **Calculated**, enter values for **c** and **n**.
- For **Constant**, enter a value (unit = m) in the field.

Primary phase (available with back diffusion)

This field is available when the **Back diffusion in primary phase** check box is selected.

Select **Automatic** (the default) or choose an available phase from the list for the primary phase. The primary phase is the phase where the back diffusion takes place. If **Automatic** is selected, the program tries to find the phase which gives the most back diffusion. To override this setting, choose a specific primary phase from the list.

Composition

This section displays after you add components to the System Definer.

Fast diffuser

This check box is available after you add components to the System Definer. Click to select the **Fast diffuser** check box to allow redistribution of this component in both the solid and liquid parts of the alloy.

Advanced Settings

Additional advanced settings are available. Click **Show advanced options** to display these options in the Configuration window.

Global minimization

By default the **Global minimization** check box is not selected. Click to select it to perform a global minimization test when an equilibrium is reached. This costs more computer time but the calculations are more robust.

Liquid phase

The default in the list is the **Liquid phase** already defined in the database.

Terminate on

Enter a value to terminate the calculation on the **Fraction of liquid phase** or at a specific **Temperature**.

Max no. of iterations

By default, the program tries 500 iterations before it gives up. As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.

Required accuracy

The default is 1.0E-6. This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.

Smallest fraction

The default is 1.0E-12. This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions.

The default value for the smallest site-fractions is 1E-12 for all phases except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as 1E-30.



In Console Mode, the default of 1E-30 for IDEAL phases is true unless you are using the command SET_NUMERICAL_LIMITS to reset an even-lower value (e.g. 1E-45, that is naturally enforced to all the phases in the system).

Approximate driving force for metastable phases

The check box is selected by default, which means the metastable phases are included in all iterations. However, these may not have reached their most favourable composition and thus their driving forces may be only approximate.

If it is important that these driving forces are correct, click to clear the check box to force the calculation to converge for the metastable phases.

Property Model Calculator

A **Property Model Calculator** enables you to predict and optimize material properties based on their chemical composition and temperature. The available calculation types are **Single**, **One Axis**, **Grid**, **Min/Max**, and **Uncertainty**. Using these, you can evaluate models simultaneously over a range of compositions and temperature and cross plot the results, then conduct an uncertainty analysis and plot the results as either a histogram or a probability plot.

- ▶ The **Configuration** window for a Property Model Calculator using the *Phase transition* model is shown and described in ["Configuration Window Settings" on page 106](#).
- ▶ There are **General Models** and **Steel Models** available. For more information, see ["About the Property Models in Thermo-Calc" on the next page](#).



You can also create custom property models. See ["Introduction to the Property Model Development Framework" on page 2](#).

Property Model Calculator Workflow

At the start when you are designing a project, it is recommended you first test it by performing a **Single** calculation type. This verifies that the configuration of the model is valid, otherwise you will get a *Not a Number* result in the ["Event Log Window" on page 203](#), which indicates the calculation did not work correctly.

Once the Single calculation performs successfully, you can experiment with other calculation types such as **Grid**, **Min/Max** or **Uncertainty**. Best practice for both Grid and Uncertainty is to start with a small number of steps (Grid) or samples (Uncertainty) to confirm that it works before increasing the number of steps or samples.

For a Grid calculation, you can additionally plot a *Heat map*, *Contour* or *3D* diagram. This setting is done on the ["Plot Renderer" on page 179](#).

In general, the workflow for each model differs. A recommended start point is to do a **One axis** calculation (using the ["Equilibrium Calculator" on page 48](#)) to determine what phases you get and where the transitions are before setting up the Property Model Calculator.

- ▶ ["The Quick Start Wizard and Templates" on page 26](#) and ["Creating a Project from a Template" on page 30](#)

About the Property Models in Thermo-Calc



The **General models** are available to all users. To run calculations with the **Steel models** (martensite and pearlite) requires a valid maintenance license plus licenses for both the TCFE9 and MOBFE4 databases.

General Models

These **General Models** are available with the ["Property Model Calculator" on the previous page](#):

- ["Coarsening Model" on page 78](#): Calculates the coarsening rate coefficient K (m^3/s) of a spherical precipitate phase in a matrix phase.
- ["Driving Force Model" on page 80](#): Calculates the thermodynamic driving force for a phase.
- ["Equilibrium Model" on page 80](#): Calculates the equilibrium for the given conditions. Optionally define additional Function definitions.
- ["Interfacial Energy Model" on page 81](#): Estimates the interfacial energy between a matrix phase and a precipitate phase using thermodynamic data from a CALPHAD database.
- ["Liquid and Solidus Temperature Model" on page 82](#): Use this to complete a common calculation. For example, with this model one can easily use uncertainty calculations, varying one or more conditions, and see how that affects the liquidus and solidus temperatures.
- ["Phase Transition Model" on page 83](#): Calculates the point when a new phase may form by varying set conditions. The model is useful to determine melting temperature, boiling temperature or solubility limits. It returns the phase transformation temperature, or composition, depending on the varied condition.
- ["Yield Strength Model" on page 84](#): Calculates yield stress. It returns the calculated yield strength at room temperature for the specified material using the equilibrium values calculated at a particular temperature and by further defining the following contributions to the total yield stress: precipitation strengthening, solid solution, grain boundary strengthening, and constant addition of strength. For details see ["About the Yield Strength Model" on page 89](#).



["About the Steel Property Models in Thermo-Calc" on page 99](#)

Calculation Types

- ▶ ["About the Uncertainty Calculations" on page 226](#) and ["Heat Map, Contour and 3D Plots" on page 217](#)

The Property Model Calculator includes these calculation types:

- **Single:** Calculates a single point.
- **One axis:** Varies a quantity on the X-axis.
- **Grid:** Evaluates two axis variables of the selected quantities in the specified range and number of steps. You can then select to create heat map, contour and 3D plots on the Plot Renderer.
- **Min/Max:** Evaluates the property model(s) for all variations of the selected quantities at the given limits. The Mean field is as defined under Condition Definitions for the respective quantity. The total minimum and maximum of the model(s) results are shown in the Event log.
- **Uncertainty calculation:** Evaluates the property model(s) where the values of the quantities are sampled from Gaussian distributions. The Mean field is as defined under Condition Definitions for the respective quantity. The result is visualized as a histogram or normal probability plot by adding a Plot Render activity.

Property Model Development Framework

With the Property Model Calculator you can now develop your own models and integrate them into Thermo-Calc. In other words, you can customize the software to meet your modeling needs.

Models are developed using the programming language Python, and model development is possible without any additional installation using a simple editor, such as Notepad++. You can also use a Python Integrated Development Environment (IDE) to access advanced features such as debugging of the property models and autocompletion.

Models are automatically encrypted for safe and secure file sharing.

- ▶ ["Introduction to the Property Model Development Framework" on page 2](#)

Examples and Video Tutorials

WEBSITE



For an introduction to the Property Model Calculator, go to the video tutorial



page on our [website](#) and under **Release and New Products**, click the arrow next to **Property Model Calculator**.

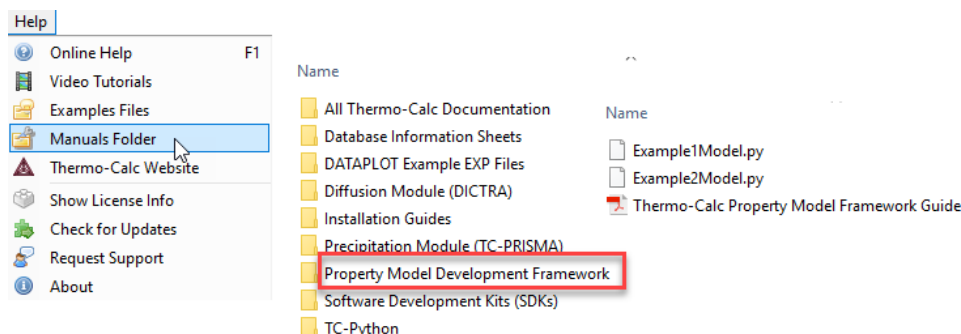
YouTube



You can also go to [YouTube](#) channel to review the available training videos. Subscribe to the channel to be updated when new videos are added. Also see the [video introduction](#) to the Property Model Calculator.

PROPERTY MODEL DEVELOPMENT FRAMEWORK PDF AND EXAMPLES

There is a PDF guide and tutorial examples included with your installation. In Thermo-Calc from the menu, select **Help → Manuals Folder**. Then double-click to open the **Property Model Development Framework** folder. This guide is also available on our [website](#).



Coarsening Model

The **Coarsening** model calculates the coarsening rate coefficient K (m^3/s) of a spherical precipitate phase in a matrix phase.



This model requires that the thermodynamic and kinetic databases used include descriptions of molar volume of the matrix and precipitates as well as mobilities for the matrix phase.



For an example of a coarsening model, see ["PM_G_02: Coarsening and Interfacial Energy" on page 267](#).

Configuration Settings

The settings are found on the ["Property Model Calculator" on page 75](#) when the **Coarsening** model is selected under **General models**.



Click the **Description** tab for more information about the model. When the property model is not encrypted or it is a user-defined property model, there is also a **Python code** tab that displays the code related to the model.

- **Matrix phase:** Choose a **Matrix phase**.
- **Precipitate phase:** Choose a **Precipitate phase** to calculate its coarsening rate.

Returns the coarsening rate coefficient [m³/s] for the precipitate phase and the interfacial energy [J/m²] between matrix and the precipitate phase.

Particle Coarsening

In the coarsening regime where the driving force is capillarity, the change of mean particle radius evolves according to the equation:

$$r^{-3} - r_0^{-3} = Kt$$

Following Morral and Purdy (1994)¹, the rate constant of precipitating β phase in a multicomponent α phase is

$$K = \frac{8\sigma V_m^\beta}{9} \left[\left[c_i^\beta - c_i^\alpha \right]^T [M]^{-1} \left[c_k^\beta - c_k^\alpha \right] \right]^{-1}$$

The mobility matrix M is not the same as the mobilities that can be obtained directly from the Diffusion Module (DICTRA). The M matrix instead corresponds to the L'' matrix as defined by Andersson and Ågren (1992)².

Using the u -fractions that is defined as

$$u_k = \frac{x_k}{\sum_{j \in S} x_j}$$

where the summation only is performed over the substitutional elements give the final equation for the coarsening rate coefficient.

1. Particle coarsening in binary and multicomponent alloys," *Scr. Metall. Mater.* 30, 905–908.

2. Models for numerical treatment of multicomponent diffusion in simple phases. *J. Appl. Phys.* 72, 1350–1355.

$$K = \frac{8\sigma V_m^\beta}{9} \left[\left[u_i^\beta - u_i^\alpha \right]^T [L_{jk}^{\prime\prime\alpha}]^{-1} \left[u_k^\beta - u_k^\alpha \right] \right]^{-1}$$

The interfacial energy σ is calculated using the extended Becker's model (that also is available as a separate Property Model Calculator model).

Driving Force Model

The **Driving Force** model calculates the thermodynamic driving force for a phase.



For an example of a driving force model, see ["PM_G_03: Driving Force and Interfacial Energy" on page 271](#).

Configuration Settings

The settings are found on the ["Property Model Calculator" on page 75](#) when the **Driving force** model is selected under **General models**.



Click the **Description** tab for more information about the model. When the property model is not encrypted or it is a user-defined property model, there is also a **Python code** tab that displays the code related to the model.

- **Matrix phase:** Choose a **Matrix phase**, the single phase region to start in. Select 'Any phase' to use the phases that take part of the initial equilibrium or choose a specific phase.
- **Precipitate phase:** Choose a **Precipitate phase** to calculate its driving force.

The calculation result is the driving force divided by RT .

Equilibrium Model

The Equilibrium model calculates the equilibrium for the given conditions.



When you use this model with the **Property Model Calculator**, it is the same calculation result as when you are using an **Equilibrium Calculator** with the **Single equilibrium** calculation type.

Configuration Settings

The settings are found on the ["Property Model Calculator" on page 75](#) when the **Equilibrium** model is selected under **General models**.



Click the **Description** tab for more information about the model. When the property model is not encrypted or it is a user-defined property model, there is also a **Python code** tab that displays the code related to the model.

Define additional **Quantity Definitions** and **Function Definitions**. All quantities that normally can be obtained from an equilibrium calculation can also be obtained when plotting the results, as well as the defined functions.

Interfacial Energy Model

Use the **Interfacial Energy** model to estimate the interfacial energy between a matrix phase and a precipitate phase using thermodynamic data from a CALPHAD database. The approximation model is based on Becker's bond energy approach and is also available in Precipitation Module (TC-PRISMA). In the actual calculation, the coefficients taken distinguish between only bcc and fcc structure for the (110) and (111) lattice plane, respectively.

For other planes and/or other phases, the estimate is approximate. In most situations, it is recommended to perform calibrations against some experimental data because the interfacial energy is dependent on so many factors that are ignored in the estimation, for example entropy, incoherency, orientation, and curvature, etc. Uncertainty factors must also be considered as thermodynamic data in CALPHAD databases are not always accurate.



For an example, see ["PM_G_02: Coarsening and Interfacial Energy" on page 267](#).

Configuration Settings

The settings are found on the ["Property Model Calculator" on page 75](#) when the **Interfacial energy** model is selected under **General models**.



Click the **Description** tab for more information about the model. When the property model is not encrypted or it is a user-defined property model, there is also a **Python code** tab that displays the code related to the model.

Select the **Matrix phase** and **Precipitate phase** to return the interfacial energy [J/m²].

Estimation of Coherent Interfacial Energy

Interfacial energy is an important parameter used in precipitation simulations to calculate the rates of nucleation, growth/dissolution, and coarsening. The value of interfacial energy can vary dramatically (usually between 0.01 to 2.0 J/m²).

The extended Becker's model functions to estimate coherent interfacial energy by using thermodynamic data from existing CALPHAD thermodynamic databases:

$$\sigma_c = \frac{n_s z_s}{N_A z_l} \Delta E_s$$

where σ_c is the coherent interfacial energy, n_s is the number of atoms per unit area at the interface, z_s is the number of cross bonds per atom at the interface, z_l is the coordination number of an atom within the bulk crystal lattice, and ΔE_s is the energy of solution in a multicomponent system involving the two phases being considered [Becker, 1938]¹.

Liquid and Solidus Temperature Model

The **Liquidus and solidus temperature** model calculates the liquid phase. If only the liquidus temperature is required, the calculation times are reduced.

Configuration Settings

The settings are found on the ["Property Model Calculator" on page 75](#) when the **Liquidus and solidus temperature** model is selected under **General models**.



Click the **Description** tab for more information about the model. When the property model is not encrypted or it is a user-defined property model, there is also a **Python code** tab that displays the code related to the model.

- **Only calculate liquidus temperature:** Select this check box as required.
- **Liquid phase:** Choose the liquid phase of the system. This is a fallback choice. Normally this should be handled automatically, even if multiple liquid phases are present.
- **Upper temperature search limit:** Initial temperature for the liquidus calculation. This needs to be in the fully liquid state.

1. Becker, 1938. 'Die Keimbildung bei der Ausscheidung in metallischen Mischkristallen', *Ann. Phys.* 424, 128–140.

-
- **Max. number of iterations:** Maximum number of phase transformation iterations performed. The default is 10.
 - **Global minimization for liquidus** and **Global minimization for solidus:** Select one or both of these check boxes to find all phases present in the equilibria. However, note it significantly increases the calculation time.



Global minimization recommendation: First try to calculate without global minimization, then if inaccuracies occur, switch global minimization on. Problems mostly occur if many phases are present at a given temperature.

- **Suspend gas phase:** The occurrence of a gas phase may mislead the liquidus temperature determination. If the presence of the gas phase is absolutely required, you can activate it and then choose a user-defined phase.
- **Gas phase:** Choose a phase from the list.

Phase Transition Model

By varying set conditions, the **Phase Transition** model calculates the point when a new phase may form. The model is useful to determine melting temperature, boiling temperature or solubility limits. It returns the phase transformation temperature, or composition, depending on the varied condition.



For an example see ["PM_G_01: Phase Transition" on page 265](#).

Configuration Settings

The settings are found on the ["Property Model Calculator" on page 75](#) when the **Phase transition** model is selected under **General models**.



Click the **Description** tab for more information about the model. When the property model is not encrypted or it is a user-defined property model, there is also a **Python code** tab that displays the code related to the model.

Define the:

- **Matrix phase:** The single phase region to start in. Select 'Any phase' to use the phases that take part of the initial equilibrium or choose a specific phase.
- **Phase to form:** For the new phase to be formed, select 'Any phase' or choose a specific phase.
- **Condition to vary:** Choose whether to vary a composition or temperature condition when calculating the phase transition.
- **Search direction:** For the composition or temperature condition being varied, choose the Search direction to be in a **Positive**, **Negative**, or **Positive and Negative** direction.



The start value (given in *Condition Definitions*) and phase transition point need to be within these limits, otherwise the model returns *Not a Number* as result. For example, a start temperature is 1100 K then the limits need to be outside these, e.g. 500-1500.

Yield Strength Model

► ["About the Yield Strength Model" on page 89](#)

The **Yield strength** model is available with the Property Model Calculator and calculates yield stress. It returns the yield strength at room temperature for the specified material using the equilibrium values calculated at temperature T . The model is defined by further setting these contributions:

- Intrinsic strength (σ_i) contribution
- Solid solution strengthening (σ_{ss})
- Grain boundary strengthening (σ_{gb})
- Precipitation strengthening (σ_p)
- Constant strength addition (σ_c)



For examples of the yield strength models, see ["PM_G_04_Yield_Strength" on page 273](#), ["PM_G_05_Yield_Strength_NiAlCr" on page 276](#), and ["PM_G_06_Yield_Strength_HEA" on page 279](#)

Configuration Settings

The settings for these contributions are found on the ["Property Model Calculator" on page 75](#) when the **Yield strength** model is selected under **General models**.



Click the **Description** tab for more information about the model. When the property model is not encrypted or it is a user-defined property model, there is also a **Python code** tab that displays the code related to the model.

General Model Settings

Composition unit

Choose a unit: **Mass percent**, **Mole percent**, **Mass fraction** or **Mole fraction**.

Condition Definitions

Choose a unit (**Kelvin**, **Celsius** or **Fahrenheit**) and then enter a value for the **Temperature** and **Composition** for each component.

The values entered in *Condition Definitions* are used as the start values for the different calculation types.

Yield Strength Model Settings

Matrix Phase

Matrix phase: Choose a **Matrix phase**.

Intrinsic and solid solution strengthening

Click to select the **Intrinsic and solid solution strengthening** check box to further define this model.

Then if required, click to select the **Specify temperature at which to evaluate solid solution strength** check box and enter a **Strength evaluation temperature** in the field. The unit of temperature is the same as that selected above under *Condition Definitions*.



If no temperature is entered, room temperature is used.

Grain boundary strengthening

Click to select the **Grain boundary strengthening** check box to include calculated grain

boundary strengthening (σ_{gb}). Then enter the following settings.

- **Grain size:** The grain diameter in μm .
- **Hall-Petch constant:** k_{h-p} in $\text{Mpa } \mu\text{m}^{1/2}$. For example, 004 for Al, 0.16 for Ni.

Precipitation strengthening

Click to select the **Precipitation strengthening** check box to include calculated precipitation strengthening (σ_p). Then enter the following settings.

Select a **Precipitate** from the list.

The precipitation strengthening contribution (σ_p) is calculated by one of these models:

Select a **Precipitation strengthening model** from the list:

- **Simplified model (general)**
- **Seidman model (Al-base):** Preferentially used for Al-based alloys.
- **Reppich model (Ni-base):** Preferentially used for Ni-based alloys.

For the **Simplified model (general)**, enter values in the fields for the following. The default values of k_p and r_c are optimized against experiments for Al-Sc.

- **Mean radius Simplified model:** The precipitate mean radius. The unit is meter (m).
- **k_p :** The prefactor for the simplified model, which adjusts the overall height of the yield strength curve.
- **Critical radius r_c ,** which determines the mean precipitate radius where transition between cutting and looping occurs. The unit is meter (m).

For the **Seidman model (Al-base)**, enter values in the fields for the following. The default parameters are optimized against experiments.

- **Mean radius Seidman model:** The precipitate mean radius. The unit is meter (m).
- **Anti-phase boundary energy: γ_{apb} ,** which is the average anti-phase boundary energy for the precipitate phase. The unit is Jm^{-2} .
- **m :** A Seidman exponent, it is a constant in the expression for strengthening by modulus mismatch.
- **α :** A Seidman prefactor. It is a fitting constant in the expression for coherency strengthening.

For the **Reppich model (Ni-base)**, enter values in the fields for the following. The default parameters are optimized against experiments.

- **Mean radius Reppich model:** The precipitate mean radius. The unit is meter (m).
- **Anti-phase boundary energy:** γ_{apb} , which is the average anti-phase boundary energy for the precipitate phase. The unit is Jm⁻².
- **w:** A parameter that accounts for elastic repulsion between strongly coupled dislocations.
- **A:** Numerical factor reflecting particle morphology (0.72 for spherical).

Constant strength addition

Enter a value for the **Constant strength addition**, σ_c . The unit is MPa.

Equilibrium minimization strategy

Select an **Equilibrium minimization strategy**.

The **Minimization strategy** setting is used to ensure that the most stable minimum under the specified conditions is computed. The default uses the **Global test preferred** option.

With either the *Global* or *Local preferred* setting, the program cycles through options before it gives up:

- For **Global test preferred** the minimization starts with a global test and if that fails it runs full global minimization.
- For **Local minimization preferred** the minimization starts with a local minimization, in case of failure it tries a global test and finally a full global minimization.

If you choose **Local minimization only** or **Global minimization only**, the program just tries the one setting and gives up if it fails.



For general information about global minimization, see the topic related to the Console Mode command, ["GLOBAL_MINIMIZATION" on page 139](#).

Calculation Type Settings

Calculation Type

Choose a calculation type: **Single** (no axes), **One axis**, **Grid**, **Min/Max** or **Uncertainty**.

- Select **Single** to calculate a single point. Any model can use this calculation type and no additional settings are required. The results from this calculation are displayed in the **Event Log** or if a **Table Renderer** is used, in the **Results** window.

▶ ["Equilibrium Model" on page 80](#)

- Select **One axis** to vary a quantity on the X-axis.
- Select a **Grid** to evaluate two axis variables of the selected quantities in the specified range and number of steps.
- The **Min/Max** calculation evaluates the property model(s) for all variations of the selected quantities at the given limits. The **Mean** field is as defined under Condition Definitions for the respective quantity. The total minimum and maximum of the model(s) results are shown in the Event log.
- The **Uncertainty** calculation evaluates the property model(s) where the values of the quantities are sampled from Gaussian distributions. The **Mean** field is as defined under Condition Definitions for the respective quantity. The result is visualized as a histogram or normal probability plot by adding a Plot Render activity.

Axis Definition

For **One axis**, select a **Quantity** to vary along the X-axis, for example, **Temperature** then enter a **Min**, **Max** and **Number of steps**.

Grid Definition Settings

Grid Definitions

For the **Grid** calculation type, define the two axes variables using the fields and menus: **Quantity**, **Min**, **Max** and **Number of steps**. The number of steps along with the minimum and maximum values for the axes define a grid. For each grid point the selected models are evaluated.



For a **Grid**, on the Plot Renderer, you can choose to plot a *Heat map*, *Contour* or *3D diagram*.

▶ ["Heat Map, Contour and 3D Plots" on page 217](#)

Min/Max Definitions

For the **Min/Max** calculation type, click to select the applicable check boxes under **Quantity to enable or disable an axis**. The **Mean** field is as defined under Condition Definitions for the respective quantity.

Enter numerical values in the **ΔMin/Max** fields to evaluate the change to the quantity. The highest and lowest value of each selected model results are shown in the Event log.

Sampling of Data from Gaussian Distributions

For the **Uncertainty** calculation type, click to select the applicable check boxes under **Quantity to vary this quantity**. The **Mean** field is for the distribution function as defined under *Condition Definitions* for the respective quantity. The default ΔMin/Max is a 95% confidence interval.

▶ ["About the Uncertainty Calculations" on page 226](#)

Sampling Parameters

For the **Uncertainty** calculation type, choose a number of **Standard deviations** where you want to **Truncate the distribution**. Choose the **Total number of samples**.

▶ ["About the Uncertainty Calculations" on page 226](#)

About the Yield Strength Model



The settings for these contributions are found on the ["Property Model Calculator" on page 75](#) when the ["Yield Strength Model" on page 84](#) is selected under **General models**.

The **Yield strength** model is a general model to estimate the yield stress of a material that considers these contributions to the overall yield stress of the material:

- Intrinsic strength (σ_i) for the pure elements,
- Grain boundary strengthening (σ_{gb}),
- Solid solution strengthening (σ_{ss}),
- Precipitation strengthening (σ_p), and
- A user set, constant strength contribution (σ_c).

The temperature (T) is used to evaluate the equilibrium state of the system, and the resulting compositions and phase fractions are subsequently used in the evaluation of mechanical properties. Below follows a short summary for each of the contributions.

INTRINSIC STRENGTH

Intrinsic strength, σ_i , is the base strength as evaluated from linear combination of the pure elements' strength. If data is missing for one or more elements a message displays in the software to indicate this. The result is normalized with respect to the sum of all mole fractions for FCC, BCC and HCP phases.

CONSTANT ADDITION OF STRENGTH

The parameter σ_c is set by the user as a constant strength addition to the material.

GRAIN BOUNDARY STRENGTHENING

The **grain boundary strengthening** σ_{gb} is the contribution to the total strength stemming from the grain boundary's ability to hinder dislocation movement described by the Hall-Petch relation [1].

The parameters you enter are the Hall-Petch constant, k_{h-p} in $\text{Mpa } \mu\text{m}^{1/2}$ (for example, 004 for Al, 0.16 for Ni), and the average grain diameter in μm .

SOLID SOLUTION STRENGTHENING



["PM_G_06_Yield_Strength_HEA" on page 279](#)

The **solution strengthening** σ_{ss} is the contribution to total strength due to the elastic strains in the crystal lattice caused by alloying elements of a lattice parameter differing from the main constituent. For the solid solution strengthening the option of evaluating the strength at any temperature is available. This option uses the phase fractions and compositions calculated at the overall equilibrium temperature. The model by Walbrühl et al. [2] is implemented.

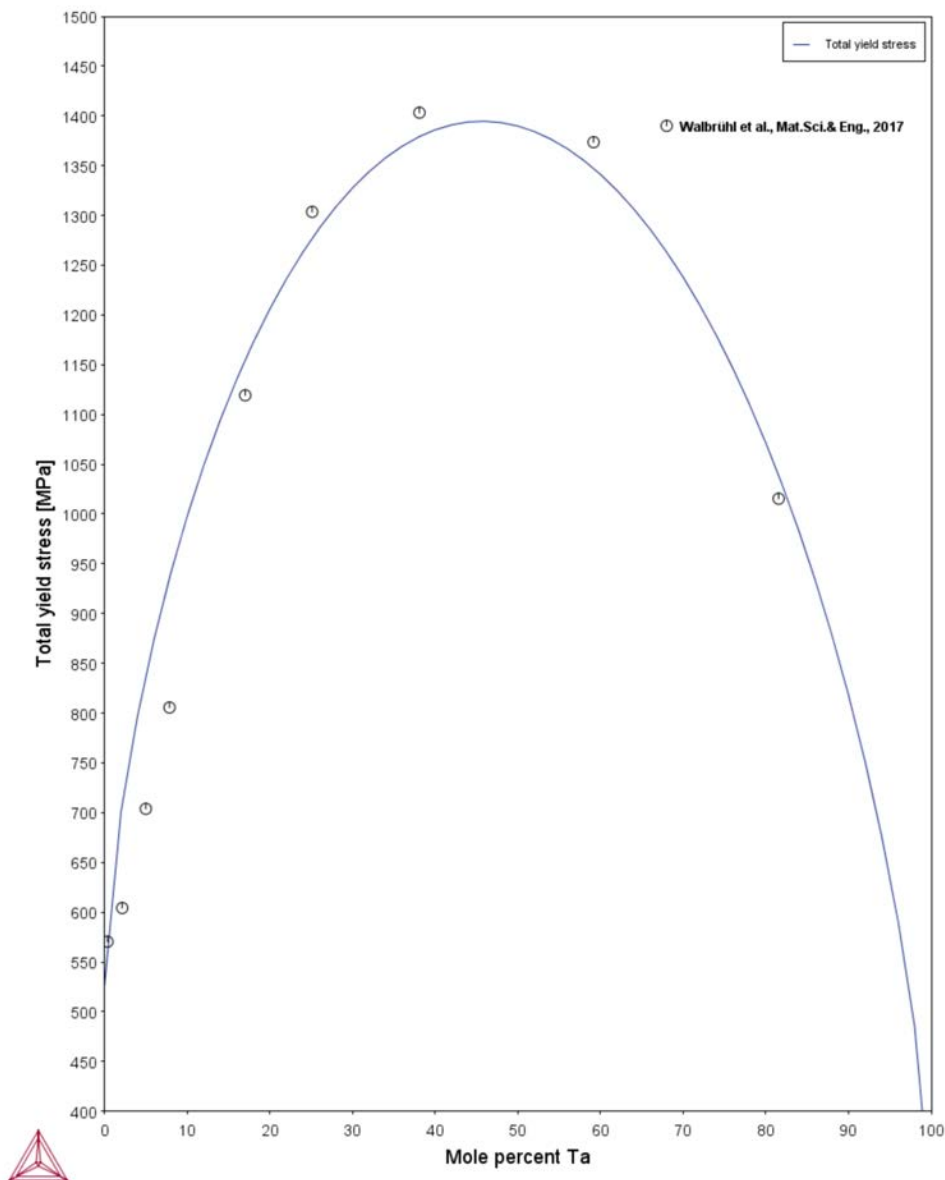


Figure 1: Yield strength vs Ta-content for the binary high entropy Mo-Ta alloy.

PRECIPITATION STRENGTHENING

The **precipitation strengthening** σ_p is the contribution to total strength due to precipitation of a secondary phase, e.g. gamma prime in Ni-base alloys or Al₃Sc precipitates in Al-base alloys. This model is available for a maximum of one precipitating phase. The following models are available to estimate the precipitation strengthening contribution.

SIMPLIFIED MODEL (GENERAL)



["PM_G_04_Yield_Strength" on page 273](#)

The **simplified model** is based on the work by Zander et al. [3] and considers the general mechanisms of cutting and looping without regard to any detailed dislocation mechanisms. The default parameters are, however, optimized against experimental data for the Al-0.3wt%Sc alloy described by Seidman et al. [4].

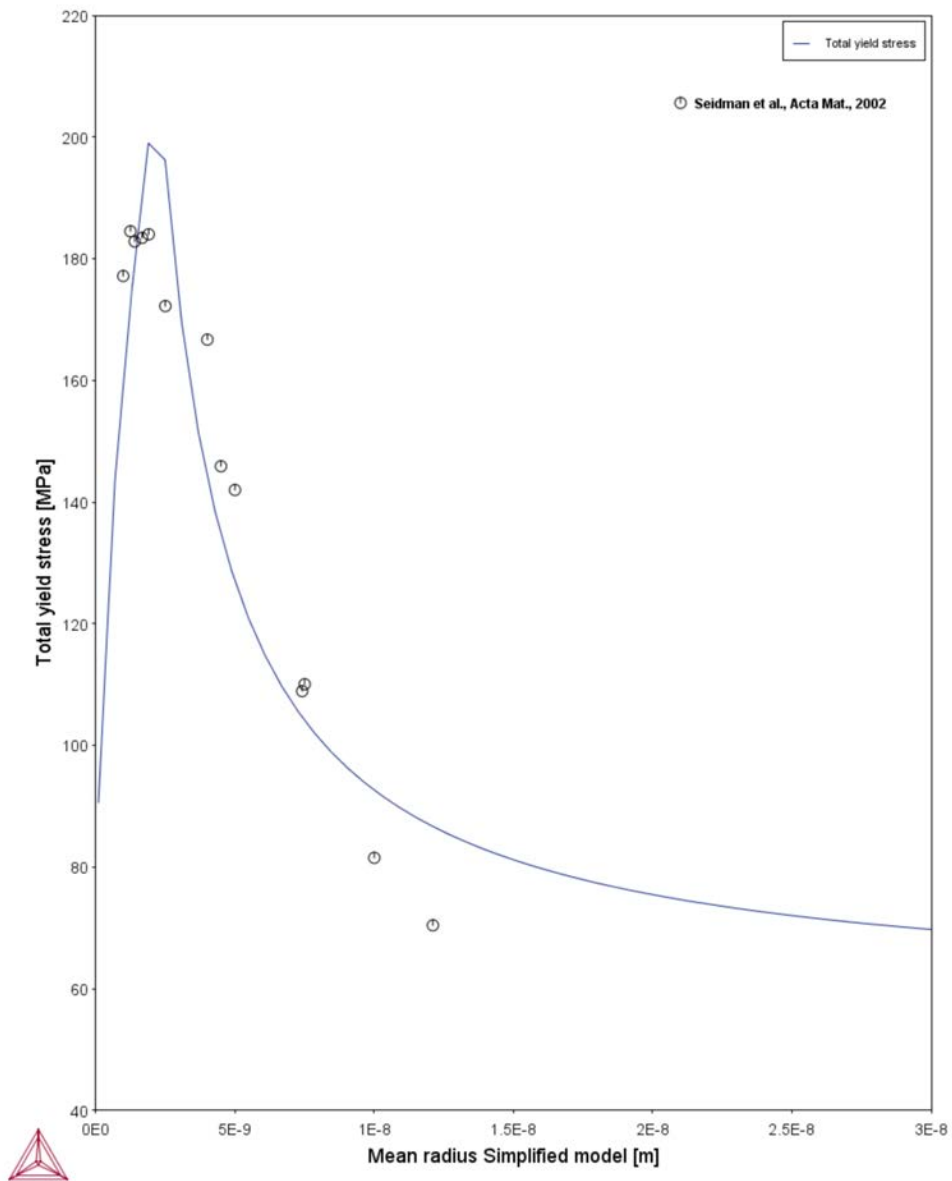


Figure 2: Simplified model

SEIDMAN MODEL (AL-BASE)



["PM_G_04_Yield_Strength" on page 273](#)

The **Seidman model (Al-base)** by Seidman et al. [4] considers several contributions to the overall precipitation strengthening - ordering, coherency stresses, shear modulus mismatch, and Orowan looping. The Seidman model is suitable for Al-base alloys with a low volume fraction of spherical precipitates. In example PM_G_04_Yield_Strength, the simplified and Seidman models are compared to experimental data on the increase in yield strength due to precipitation hardening. Although the experimental set up was designed to eliminate grain boundary and solid solution strengthening, these are also included by optimizing of model parameters.

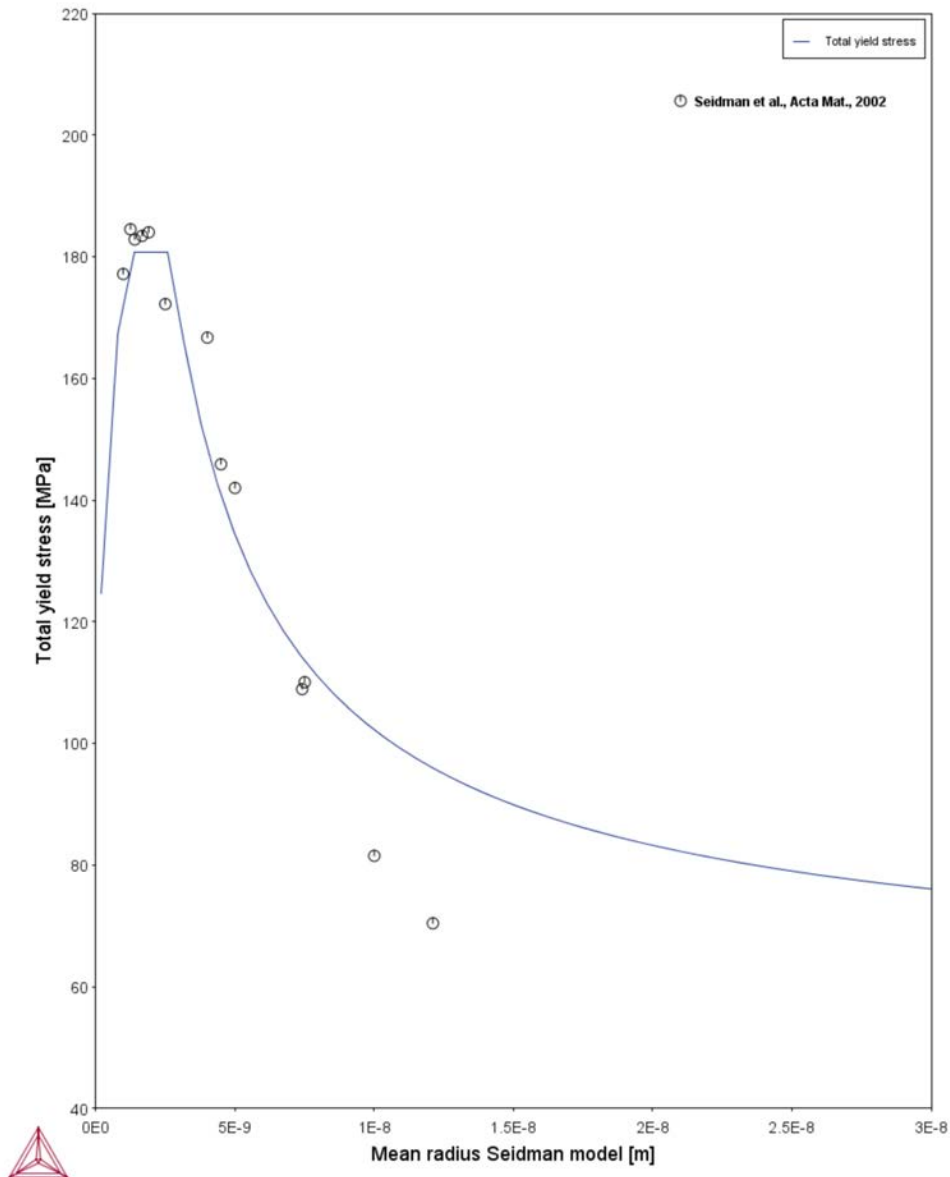


Figure 3: Seidman model [4]

REPPICH MODEL (NI-BASE)



["PM_G_05_Yield_Strength_NiAlCr" on page 276](#)

The **Reppich model (Ni-base)** by Reppich et al. [5] considers both weak and strong coupling of dislocation as they propagate through an ordered secondary phase and is thus suitable for Ni-base alloys with relatively high volume fractions of gamma prime or gamma double prime.

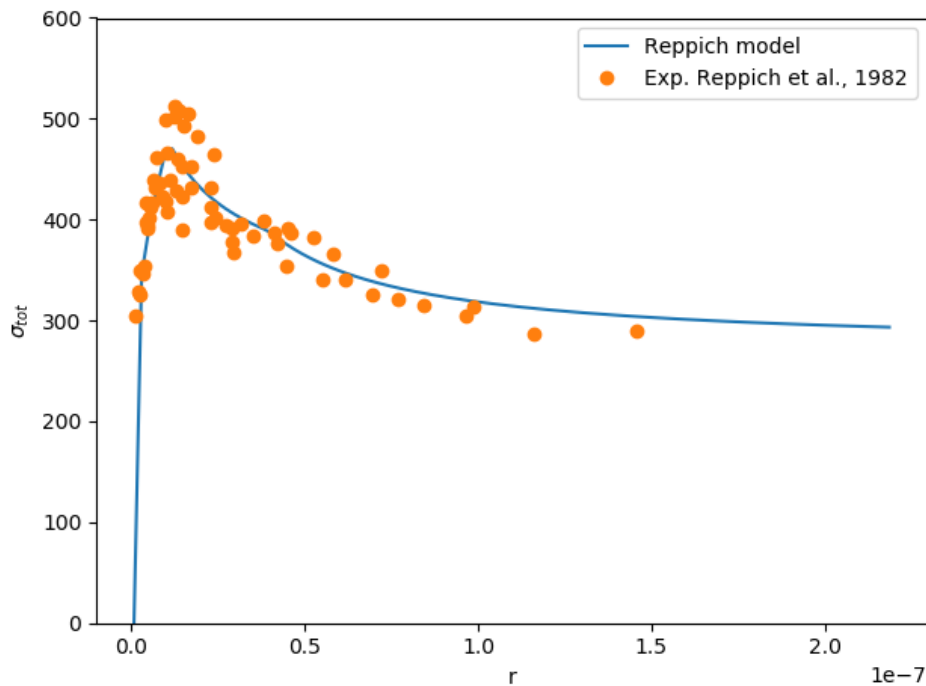


Figure 4: Reppich model plotted with results and experimental data for PE16 [6], all data is normalized with the square root of the volume fraction of precipitate.

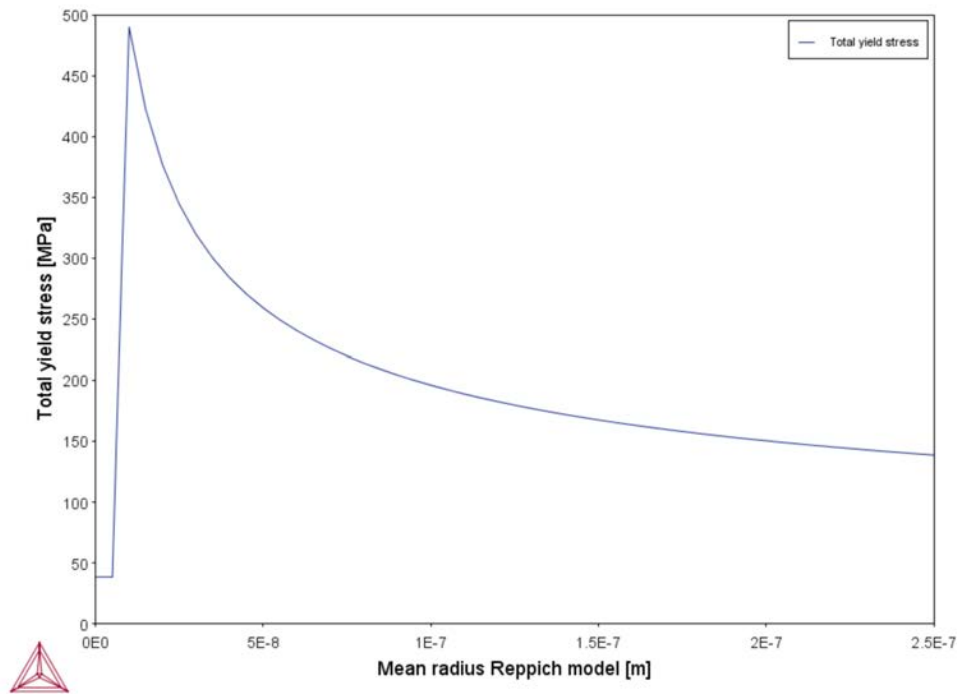


Figure 5: Reppich model yield strength vs mean precipitate radius for Ni-10Cr-10Al.

REFERENCES

1. Hansen, Niels. 2004. "Hall–Petch Relation and Boundary Strengthening." *Scripta Materialia* 51 (8): 801–6. <https://doi.org/10.1016/j.scriptamat.2004.06.002>.
2. Walbruhl, Martin, David Linder, John Ågren, and Annika Borgenstam. 2017. "Modelling of Solid Solution Strengthening in Multicomponent Alloys." *Materials Science and Engineering: A* 700 (July): 301–11. <https://doi.org/10.1016/j.msea.2017.06.001>.
3. Zander, Johan, and Rolf Sandström. 2008. "One Parameter Model for Strength Properties of Hardenable Aluminium Alloys." *Materials & Design* 29 (8): 1540–48. <https://doi.org/10.1016/j.matdes.2008.02.001>.
4. Seidman, David N., Emmanuelle A. Marquis, and David C. Dunand. 2002. "Precipitation Strengthening at Ambient and Elevated Temperatures of Heat-Treatable Al(Sc) Alloys." *Acta Materialia* 50 (16): 4021–35. [https://doi.org/10.1016/S1359-6454\(02\)00201-X](https://doi.org/10.1016/S1359-6454(02)00201-X).

5. Reppich, Bernd. 1982. "Some New Aspects Concerning Particle Hardening Mechanisms in γ' Precipitating Ni-Base Alloys—I. Theoretical Concept." Acta Metallurgica 30 (1): 87–94. [https://doi.org/10.1016/0001-6160\(82\)90048-7](https://doi.org/10.1016/0001-6160(82)90048-7).
6. Reppich, Bernd, Peter Schepp, and Günter Wehner. 1982. "Some New Aspects Concerning Particle Hardening Mechanisms in γ' Precipitating Nickel-Base Alloys—II. Experiments." Acta Metallurgica 30 (1): 95–104. [https://doi.org/10.1016/0001-6160\(82\)90049-9](https://doi.org/10.1016/0001-6160(82)90049-9).

About the Steel Property Models in Thermo-Calc



The **General models** are available to all users. To run calculations with the **Steel models** (martensite and pearlite) requires a valid maintenance license plus licenses for both the TCFE9 and MOBFE4 databases.

These **Steel Models** are available with the ["Property Model Calculator" on page 75](#). The following are part of the Steel Model Library:

- ["Martensite Fractions Model" below](#): Calculates the fraction of athermal martensite based on available driving force.
- ["Martensite Temperatures Model" on the next page](#): Calculates the martensite start and finish temperature based on modeling of the transformation barrier.
- ["Pearlite Model" on page 102](#): Calculates the thermodynamics and kinetics of pearlite formation from austenite during isothermal heat treatment.



["Steel Library TTT Diagram Template" on page 33](#) and ["Plot Settings: TTT Mode" on page 185](#)

Martensite Fractions Model



To run calculations with the **Steel models** (martensite and pearlite) requires a valid maintenance license plus licenses for both the TCFE9 and MOBFE4 databases.



For an example see ["PM_Fe_01: Fe-Cr-C Martensite with Intercritical Annealing" on page 281](#).

The **Martensite Fractions** property model calculates fraction of athermal martensite based on an analytical equation derived in Huyan et al. (2016). It is assumed that the first forming martensite morphology is the only forming one. The first morphology is determined based on the Ms-temperatures of all morphologies. This model is part of the Steel Model Library.

REFERENCE

Huyan, Fei, Peter Hedström, Lars Höglund, and Annika Borgenstam. 2016. "A Thermodynamic-Based Model to Predict the Fraction of Martensite in Steels." Metallurgical and Materials Transactions A 47 (9). 4404–10. doi:10.1007/s11661-016-3604-6.

Quantities to set in the **Property Model Calculator**:

- **Intercritical annealing**: Select **No** if the specified composition is used directly; select **Yes** to assume intercritical annealing. If you choose **Yes**, an equilibrium calculation is performed at the specified temperature and the composition of the austenite phase is used for the martensite temperature calculation.
- Enter an **Annealing temperature**.
- **Grain size [μm]**: Enter the grain size of the austenite phase in μm . By default 100 μm is set. The Ms temperature and martensite fractions change for significantly smaller grain sizes.
- **Parent phase Gibbs energy addition [J/mol]**: Enter a value in J/mol to add a Gibbs energy offset to the parent austenite phase. This can be used, for example, to correct database offsets. The default is 0 J/mol.

Axis variables you can choose on the **Plot Renderer** for the conditions defined on the Property Model Calculator:

- **Total martensite percentage**
- **Retained austenite percentage**

Martensite Temperatures Model



To run calculations with the **Steel models** (martensite and pearlite) requires a valid maintenance license plus licenses for both the TCFE9 and MOBFE4 databases.



For an example see ["PM_Fe_01: Fe-Cr-C Martensite with Intercritical Annealing" on page 281](#) and ["PM_Fe_02: Fe-Mn Martensite Morphologies" on page 283](#).

The **Martensite Temperatures** property model calculates the martensite start temperature (Ms) based on modeling the transformation barrier with fitted analytical equations. The model is based on Stormvinter et al. (2012) with subsequent update and extension by Gulapura Hanumantharaju (2018) and Thermo-Calc internal assessment. The partitionless equilibrium temperature T₀ is calculated using the thermodynamic database. The model also gives temperatures corresponding to 50%, 90%, and 99% transformations. Martensite fractions are calculated with the same algorithm as in the **Martensite Fractions** property model. This model is part of the Steel Model Library.

► ["Steel Library TTT Diagram Template" on page 33](#) and ["Plot Settings: TTT Mode" on page 185](#)

REFERENCES

Stormvinter, Albin, Annika Borgenstam, and John Ågren. 2012. "Thermodynamically Based Prediction of the Martensite Start Temperature for Commercial Steels." *Metallurgical and Materials Transactions A* 43 (10): 3870–79.

Gulapura Hanumantharaju, A. K. 2018. "Thermodynamic Modelling of Martensite Start Temperature in Commercial Steels". Master's Thesis, KTH Royal Institute of Technology, <http://urn.kb.se/resolve?urn=urn:nbn:se:kth:diva-221719>.

Quantities to set in the **Property Model Calculator**:

- **Intercritical annealing**: Select **No** if the specified composition is used directly; select **Yes** to assume intercritical annealing. If you choose **Yes**, an equilibrium calculation is performed at the specified temperature and the composition of the austenite phase is used for the martensite temperature calculation.
- **Grain size [μm]**: Enter the grain size of the austenite phase in μm. By default 100 μm is set. The Ms temperature and thus the martensite fractions change for significantly smaller grain sizes.
- **Parent phase Gibbs energy addition [J/mol]**: Enter a value in J/mol to add a Gibbs energy offset to the parent austenite phase. This can be used, for example, to correct database offsets. The default is **0** J/mol.

Axis variables you can choose on the **Plot Renderer** for the conditions defined on the Property Model Calculator:

- **Ms**: Martensite start temperature
- **Lath Ms**: Martensite start temperature of lath alpha or alpha-prime martensite
- **Plate Ms**: Martensite start temperature of plate alpha or alpha-prime martensite
- **Epsilon Ms**: Martensite start temperature of epsilon martensite

- **M50**: 50% martensite temperature
- **M90**: 90% martensite temperature
- **M99**: 99% martensite temperature

Pearlite Model



To run calculations with the **Steel models** (martensite and pearlite) requires a valid maintenance license plus licenses for both the TCFE9 and MOBFE4 databases.



With the TCFE9 database, the included elements in the pearlite model are Fe (dependent element), C, Mn, Cr, Mo, W, Si, Al, Ni, Co. Other elements are neglected by weight percent.



For an example see ["PM_Fe_03: Fe-C-Mn Pearlite" on page 284](#).



["Steel Library TTT Diagram Template" on page 33](#) and ["Plot Settings: TTT Mode" on page 185](#)

The **Pearlite** property model describes the thermodynamics and kinetics of pearlite formation from austenite. It is assumed that the overall composition of pearlite is the same as the austenite composition (system composition), and growth rate is constant over time. Growth rate and lamellar spacing of pearlite are determined by a criterion where either growth rate or Gibbs energy dissipation rate is maximized. The model considers Gibbs energy dissipation due to formation of ferrite-cementite interface in pearlite, finite austenite-pearlite interfacial mobility, solute drag (Cahn, 1962), and diffusion of elements within austenite and along austenite-pearlite interface.



Pearlite growth with preexisting ferrite or carbide or any other phase is not considered. Divergent pearlite, of which growth rate and lamellar spacing change with time, is not considered. This model only considers the transformation from FCC_A1 phase to pearlite consisting of BCC_A2 and CEMENTITE. Pearlite with other phases is not implemented.

Pearlite is assumed to nucleation on austenite grain boundaries. Grain boundary nucleation rate is modeled as a function of composition and temperature. The isothermal transformation kinetics follows Cahn (1956). Start, half, and finish times are taken as 2%, 50%, and 98% transformation, respectively.

Model parameters have been determined from published data of maximal growth rate, minimal lamellar spacing, partition coefficients, and isothermal transformation kinetics in ternary and multicomponent systems. A detailed description of the model will be published. This model is part of the Steel Model Library.

REFERENCES

Cahn, John W. 1962. "The Impurity-Drag Effect in Grain Boundary Motion." *Acta Metallurgica*, 10 (9): 789–98. doi:10.1016/0001-6160(62)90092-5.

Cahn, John W. 1956. "The Kinetics of Grain Boundary Nucleated Reactions." *Acta Metallurgica*, 4 (5): 449–59. doi:10.1016/0001-6160(56)90041-4.

Quantities to set on the **Property Model Calculator**:

- **Criterion:**
 - **Maximize growth rate:** Pearlite growth rate is maximized with respect to lamellar spacing (and for optimal pearlite, partition coefficients of substitutional alloying elements between ferrite and cementite). The calculation will give maximal growth rate and minimal lamellar spacing. This is the default criterion.
 - **Maximize Gibbs energy dissipation rate** Gibbs energy dissipation rate is maximized with respect to lamellar spacing (and for optimal pearlite, partition coefficients of substitutional alloying elements between ferrite and cementite). The calculation will give a smaller growth rate than the maximal, and a larger lamellar spacing than the minimal, which may better represent the average growth rate and lamellar spacing of all pearlite colonies in the material.
- **Pearlite mode:**
 - **Optimal pearlite:** The partitioning of substitutional alloying elements between ferrite and cementite is optimized according to the **Criterion** while keeping carbon equilibrium between the two phases. This is the default mode. This mode realizes a smooth transition between ortho-pearlite and para-pearlite.
 - **Para-pearlite:** Ferrite and cementite are in para-equilibrium where substitutional alloying elements do not partition and carbon reaches equilibrium.
 - **Ortho-pearlite:** Ferrite and cementite are in ortho-equilibrium.
- **Grain size [μm]:** Enter the austenite grain size in μm. By default 100 μm is set.

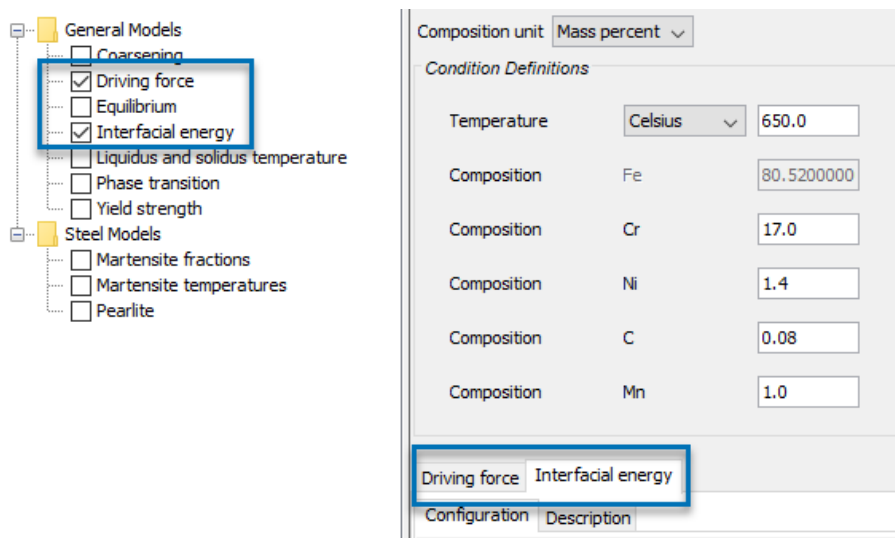
Axis variables you can choose on the **Plot Renderer** for the conditions defined on the Property Model Calculator:

- **Growth rate**
- **Lamellar spacing**
- **Cementite molar fraction in pearlite**
- **Driving force of pearlite formation**
- **Start time (2% pearlite)**
- **Half time (50% pearlite)**
- **Finish time (98% pearlite)**

Define the Property Model Calculator

1. Add a **Property Model Calculator** node to the System Definer. If you used the **Property Model Calculation** template, click the node to display the **Configuration** settings window.
2. From the left side of the **Configuration** window, click to select one or more of the check boxes under the **General Models** or **Steel Models** folders.
 - ▶ Steel models are only available if you have a license. Go to [our website](#) for more information about the Steel Model Library.

A tab with the same name as the property model opens in the right side of the window under *Condition Definitions*. When you select more than one model, a matching tab is added in the same order that the check box is selected.



3. Enter the settings described in "[Configuration Window Settings](#)" on the next page and for each *Calculation Type* (Single, Grid, Min/Max, and Uncertainty).
4. For each model on the **Configuration** tab, select or enter settings as required.



Click the **Description** tab for more information about the model. When the property model is not encrypted or it is a user-defined property model, there is also a **Python code** tab that displays the code related to the model.

5. Once you have finished defining the Property Model Calculator, you also choose settings on the ["Plot Renderer" on page 179](#).

Configuration Window Settings

An example of the Configuration window settings when using a Phase transition model and an Uncertainty calculation type.

Composition unit

Choose a unit: **Mass percent**, **Mole percent**, **Mass fraction** or **Mole fraction**.

Condition Definitions

Choose a unit (**Kelvin**, **Celsius** or **Fahrenheit**) and then enter a value for the **Temperature** and **Composition** for each component.

The values entered in *Condition Definitions* are used as the start values for the different calculation types.

Define the property model

For each property model chosen, select or enter **Configuration** settings as required.

- ▶ For links to each model with the settings details, see ["About the Property Models in Thermo-Calc" on page 76](#).



Click the **Description** tab for more information about the model. When the property model is not encrypted or it is a user-defined property model, there is also a **Python code** tab that displays the code related to the model.

Calculation Type

Choose a calculation type: **Single** (no axes), **One axis**, **Grid**, **Min/Max** or **Uncertainty**.

- Select **Single** to calculate a single point. Any model can use this calculation type and no additional settings are required. The results from this calculation are displayed in the **Event Log** or if a **Table Renderer** is used, in the **Results** window.
▶ ["Equilibrium Model" on page 80](#)
- Select **One axis** to vary a quantity on the X-axis.
- Select a **Grid** to evaluate two axis variables of the selected quantities in the specified range and number of steps.
- The **Min/Max** calculation evaluates the property model(s) for all variations of the selected quantities at the given limits. The **Mean** field is as defined under Condition Definitions for the respective quantity. The total minimum and maximum of the model(s) results are shown in the Event log.
- The **Uncertainty** calculation evaluates the property model(s) where the values of the quantities are sampled from Gaussian distributions. The **Mean** field is as defined under Condition Definitions for the respective quantity. The result is visualized as a histogram or normal probability plot by adding a Plot Render activity.

Axis Definition

For **One axis**, select a **Quantity** to vary along the X-axis, for example, **Temperature** then

enter a **Min**, **Max** and **Number of steps**.

Grid Definitions

For the **Grid** calculation type, define the two axes variables using the fields and menus: **Quantity**, **Min**, **Max** and **Number of steps**. The number of steps along with the minimum and maximum values for the axes define a grid. For each grid point the selected models are evaluated.



For a **Grid**, on the Plot Renderer, you can choose to plot a *Heat map*, *Contour* or *3D diagram*.

▶ ["Heat Map, Contour and 3D Plots" on page 217](#)

Min/Max Definitions

For the **Min/Max** calculation type, click to select the applicable check boxes under **Quantity to enable or disable an axis**. The **Mean** field is as defined under Condition Definitions for the respective quantity.

Enter numerical values in the Δ **Min/Max** fields to evaluate the change to the quantity. The highest and lowest value of each selected model results are shown in the Event log.

Sampling of Data from Gaussian Distributions

For the **Uncertainty** calculation type, click to select the applicable check boxes under **Quantity to vary this quantity**. The **Mean** field is for the distribution function as defined under *Condition Definitions* for the respective quantity. The default Δ Min/Max is a 95% confidence interval.

▶ ["About the Uncertainty Calculations" on page 226](#)

Sampling Parameters

For the **Uncertainty** calculation type, choose a number of **Standard deviations** where you want to **Truncate the distribution**. Choose the **Total number of samples**.

▶ ["About the Uncertainty Calculations" on page 226](#)

Diffusion Calculator



The Diffusion Calculator is available with three elements if you do not have the additional Diffusion Module (DICTRA) license. With the add-on module you can use all available elements as per the licensed database selected. See ["Available Graphical Mode Features" below](#) for details.

A **Diffusion Calculator** allows you to set the conditions for, and perform, a diffusion calculation. You can add the calculator to the System Definer directly (right-click and select it from the **Create New Successor** menu) or use the **Diffusion Simulation** template.

Once you have added a Diffusion Calculator, the **Configuration** window has these settings tabs:

- **Conditions:** Set the conditions for your calculation that define the geometry, regions, phases, grids, composition profiles and the thermal profile.
- **Options:** Modify the simulation conditions such as the choosing the default solver (automatic or homogenization) and the time integration method. Also define the time step controls and if you choose homogenization as the solver, define further settings such as the interpolation scheme and whether to use global minimization or not.

Available Graphical Mode Features

The Diffusion Module is an add-on module to the core Thermo-Calc software.



A separate license is required to perform calculations for more than three elements. Without it you are able to use the module in *Demo Mode*. This is not available in Console Mode. See ["Demonstration \(Demo\) Mode" on page 111](#) to learn more.

DIFFUSION SIMULATION TEMPLATE

A **Diffusion Simulation** template is available to all Thermo-Calc users when in Graphical Mode.

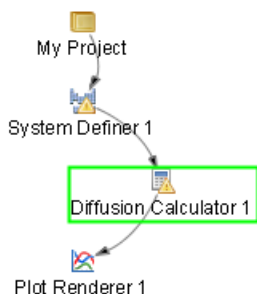


If you are using the Diffusion Module in Demo Mode, see ["Demonstration \(Demo\) Mode" on page 111](#) for what is available to you. Even if you have a license, you may find yourself in Demo Mode if you have a network license and all the licenses are checked out.

Using the Template

When you first open Thermo-Calc in Graphical Mode, on the **My Project** window, click the **Diffusion Simulation** button to add a *System Definer*, *Diffusion Calculator* and *Plot Renderer* to the **Project** tree.

Click the **Diffusion Simulation** icon in the Templates window to add **THESE NODES** to the Project.



► ["Creating a Project from a Template" on page 30.](#)

DIFFUSION CALCULATOR

A Diffusion Calculator allows you to set the conditions for your calculation that define the geometry, regions, phases, grids, composition profiles and the thermal profile, plus additional options. Many of the settings are automatically set as you define your system. Details about this activity are described in ["Diffusion Calculator" on the previous page](#).

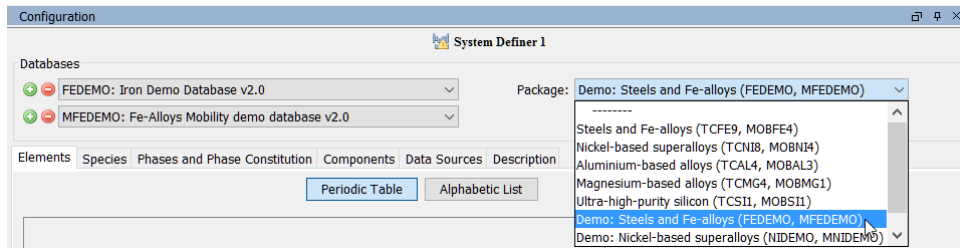
DEMO DATABASE PACKAGES FOR THE EXAMPLES COLLECTION

Both a thermodynamic and mobility database are required to run the Diffusion Module simulation. If you have a Diffusion Module (DICTRA) license you can run all the examples because the demonstration database packages are included with your installation.

Select the database packages from the **System Definer Configuration** window to run a simulation.



If you are in Demo Mode, see ["Demonstration \(Demo\) Mode" on the next page](#) to learn more.



DEMONSTRATION (DEMO) MODE

The Diffusion Module and some examples are available to all Thermo-Calc users but only for simulations with three elements. If you do not have a license for then you are in *Demo Mode* when using the Diffusion Calculator or Diffusion Simulation template.

Diffusion Simulation Template

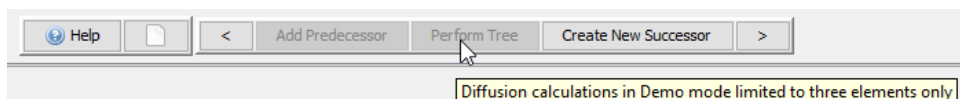
When you are in DEMO mode, in the **Templates** area this is indicated by the text under the logo.



Diffusion Calculator

If you are experimenting with the Diffusion Calculator in Demo Mode, you may have access to a variety of databases based on your license. However, you can only define three elements for a demo simulation.

If you define more than three elements on the System Definer, when you go to the Diffusion Calculator, the **Perform** button is unavailable and the tooltip explains why.

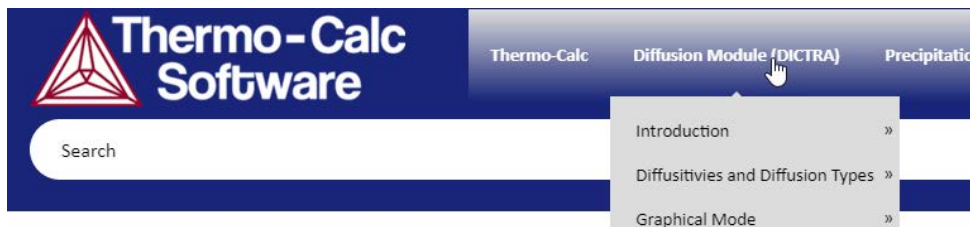


Even if you have more than three elements, the Plot Renderer **Perform** button is still available. However, if you click the button and try to run the simulation the Event Log displays an error message.

Define the Diffusion Calculator

▶ ["Available Graphical Mode Features" on page 109](#)

Working with diffusion simulations is an advanced topic. It is recommended you review the Diffusion Module (DICTRA) documentation and videos available or search for a specific topic.



1. Add a **Diffusion Calculator** node to the System Definer. If you used the **Diffusion Simulation** template, click the node to display the **Configuration** settings window.
2. In the Diffusion Calculator **Configuration** window, enter the settings described in ["Conditions Tab Settings" below](#) and ["Options Tab Settings" on page 121](#).
3. Once you have finished defining the Diffusion Calculator, you also choose settings on the ["Plot Renderer" on page 179](#). Some additional settings are specific to the ["Diffusion Calculator Plot Renderer" on page 185](#).

Conditions Tab Settings

The following Configuration window is from the *Graphical Mode Quick Start Guide*. It is using project example file *D_07: Diffusion Carburization Multiphase*.

The screenshot shows the 'Configuration' window for a 'Carburization multiphase' simulation. The 'Conditions' tab is active, showing various settings for the simulation.

- Composition unit:** Mass percent
- Length unit:** m
- Geometry:** Planar
- Austenite:** A horizontal bar representing the austenite phase.
- Left Interface Boundary:**
 - Show left interface boundary
- Region:**
 - Name: Austenite
 - Width: 0.003 m 100 points and type Geometric Ratio: 1.02
 - Phase: FCC_A1
 - Phase: M7C3
 - Phase: M3C2
 - Composition profiles: Edit
- Right Interface Boundary:**
 - Show right interface boundary
- Left Boundary Condition:**
 - Mixed zero flux and activity
 - Activity: 1.0
 - Zero flux
- Right Boundary Condition:**
 - Closed system
- Thermal Profile:**
 - Isothermal (selected)
 - Non-isothermal
 - Temperature: 1123.0 Kelvin
 - Simulation time: 1000.0 Hours

At the bottom, there are navigation buttons: Help, Add Predecessor, Perform Tree, Create New Successor, and a right arrow.

These are the settings available from the **Conditions** tab. To edit the defaults for some settings, go to **Tools → Options → Graphical Mode → Diffusion**.



The Diffusion Module (DICTRA) in Console Mode has commands to perform some of the settings also available on the Diffusion Calculator. Where possible the name of the command is indicated and includes a link to the topic.

General

COMPOSITION UNIT

Choose from **Mass percent**, **Mole percent**, **Mass fraction** or **Mole fraction**.

LENGTH UNIT

Choose **m**, **μm** or **nm**.

GEOMETRY

Choose **Planar**, **Spherical** or **Cylindrical**. For Cylindrical, also enter a value for the **First interface position**.

With a cylindrical or spherical geometry, the system's zero coordinate (left boundary) is at the centre of the cylinder or sphere. The highest coordinate (right boundary) is defined by the cylinder or sphere radius.



Region Settings



There should be one unique phase in each region.

LEFT AND RIGHT INTERFACE BOUNDARY

Toggle between hiding and showing the **Left interface boundary** or **Right interface boundary**.

Click the **Add quantity**  or **Remove quantity**  buttons as required to add a **Phase** and then enter a value for the **Driving force** as required. The default driving force is $1.0\text{E-}5$.

NAME

Enter a **Name** for the region in the field. For example, enter `Austenite`. This name is automatically updated on the tab and above the grid points graphic. You can also double-click the tab to enter the name.

WIDTH

Enter a numerical value in the **Width** field. The unit is the one selected for the **Length unit**.

POINTS

Enter a numerical value in the **points** field. The default is 50.

TYPE (OF GRID)

Select a type of grid, **Linear**, **Geometric** or **Double geometric**.

Choose **Geometric** for a grid that yields a varying density of grid points in the region. Then enter a **Ratio** to determine the distribution. A geometrical factor larger than one yields a higher density of grid points at the lower end of the region and a factor smaller than one yields a higher density of grid points at the upper end of the region.

Choose **Double geometric** to have a high number of grid points in the middle or at both ends of a region. Then specify two geometrical factors, the **Upper ratio** for the distribution in the lower (left) part of a region, and **Lower ratio** for the distribution in the upper (right) part of a region.

PHASE

Choose a **Phase** from the list. The available options are defined in the System Definer. At least one phase that dissolves all system elements must be selected.

Click the **Add quantity**  or **Remove quantity**  buttons as required.

COMPOSITION PROFILE

Click **Edit** to open the **Initial Composition** window.

Select a **Dependent component** for which the composition does not need to be given. The available options depend on the phase description.

For each **Component** choose one of these options:

- **Linear**: Enter numerical values in the **from** and **to** fields.
- **Step**: Enter numerical values in the **from** , **to** , and **step at** fields. The unit is the same as the **Length unit** selected at the top of the Configuration window.
- **Function**: Enter a composition function in the field using SI units. The syntax to use for writing functions is a Python syntax (a programming language). Any valid Python expression that is a function of the distance variable x will work.

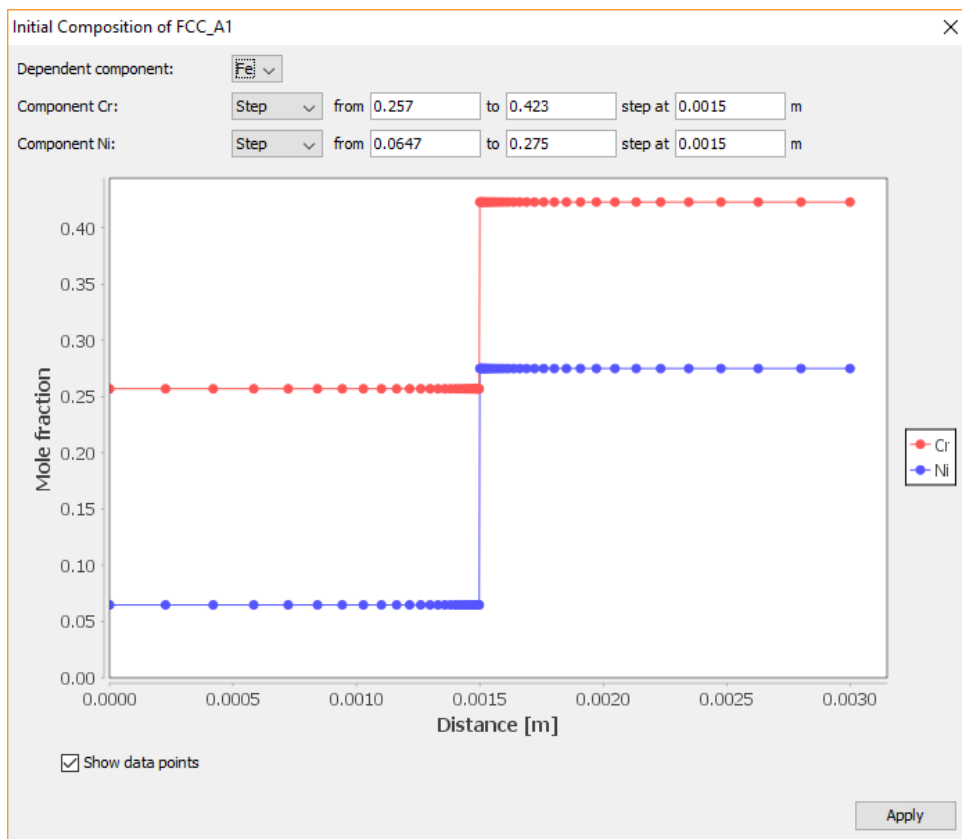


You can use the standard Jython math library but you must prefix these functions with the text "math" For example: `10 + math.sin(x*2)`. The Jython math library is available here:
<http://www.jython.org/docs/library/math.html>.

- The error function `erf(x)` is also available in the Jython math library and can be called with `math.erf(x)`.
- Another useful function is the Heaviside step-function `hs(x)`. For example, `3+2hs(x-1e-4)` provides a concentration of 3 at the left side and 5 at the right side with a sharp step in the concentration profile at $1e-4m=100mm$.

Click **Apply** when you are done.

As you add these settings, the plot helps you visualize the region based on whether you use a **Linear**, **Step** or **Function** to define the components.



Boundary Conditions

Boundary conditions are conditions that define how matter behaves at the boundaries of your system. By default, matter is not allowed to cross the system boundaries.

You can change the setting for both the lower boundary (left side/centre) and the upper boundary (right side/surface) of the system.



Examples D_06 and D_07 use boundary conditions, as described in ["Diffusion Module \(DICTRA\) Graphical Mode Examples"](#) on page 308.

The boundary condition settings are done on the **Diffusion Calculator**. The following describes the options available for the *Left boundary* and *Right boundary* conditions.

CLOSED SYSTEM

By default it is a **Closed system**. Choose **Mixed zero flux and activity** or **Composition** if the system is not closed. Corresponds to a fix flux value, which is set to zero at all times. This is the default boundary condition.

COMPOSITION

Allows the user to set a fix composition at the boundary.



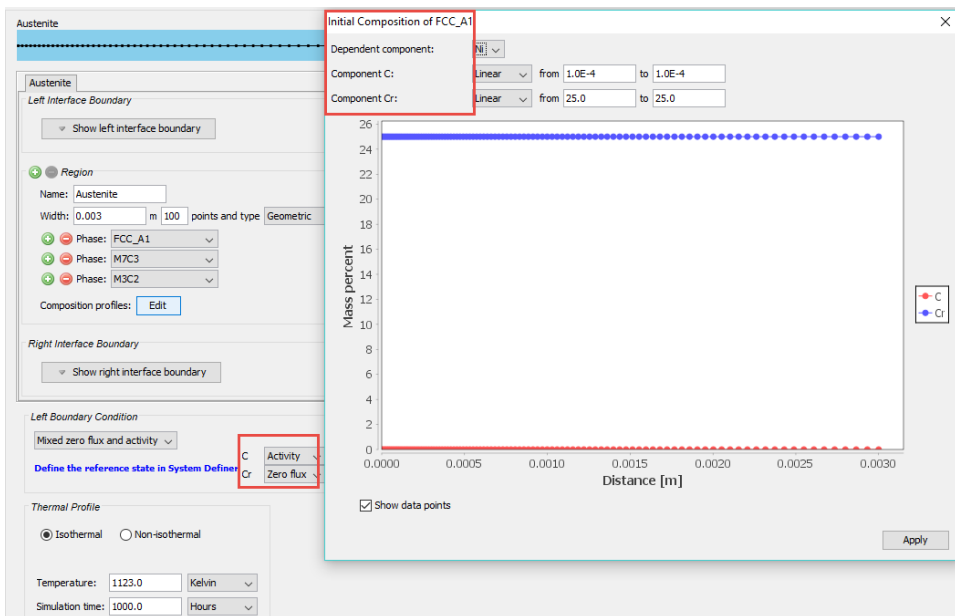
In Console Mode this is similar to the command `STATE_VARIABLE_VALUE`, but in Graphical Mode this condition is limited to setting a fixed composition.

MIXED ZERO FLUX AND ACTIVITY

The flux of selected components is either set to zero or a prescribed activity value.

For **Mixed zero flux and activity**, and for each independent element selected in the **Composition profile**, choose either **Zero flux** or **Activity** from the lists and enter a value in the field when **Activity** is selected. The reference state for the components are taken from the System Definer **Components** tab.

This image is from example *D_07: Diffusion Carburization Multiphase*.



Thermal Profile

ISOTHERMAL

Use an **Isothermal** calculation type to do a diffusion simulation at constant temperature. Choose a unit of measurement and enter a numerical value for the **Temperature** and

Simulation time.

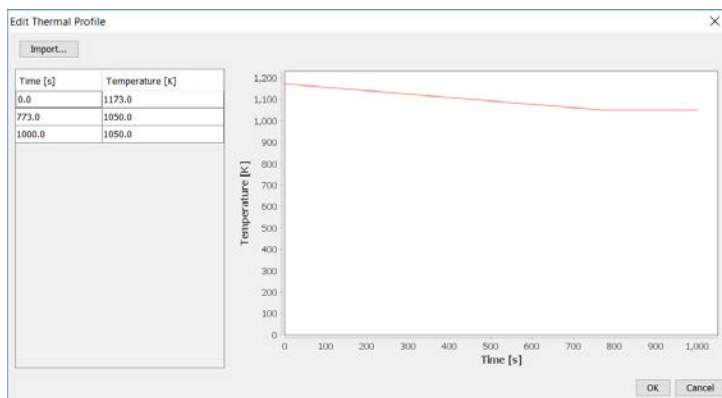
NON-ISOTHERMAL

Use a **Non-isothermal** calculation type to do a diffusion simulation with a user-defined temperature profile. Select a **Temperature unit** and **Time unit** from the lists. Enter a numerical value for the **Simulation time**.

Click **Edit thermal profile** to enter thermal profile **Temperature** and **Time** coordinates into a table. A minimum of two points is required. You can also **Import** to add your own **Thermal profile** from a text file in *.xls, *.xlsx, or *.csv formats.

EDIT THERMAL PROFILE WINDOW

This image is from example *D_04: Diffusion Fe-C Moving Boundary Austenite to Ferrite*.



Options Tab Settings

The following settings are available on the **Options** tab for a ["Diffusion Calculator" on page 109](#).



You can edit the defaults for some of these settings by going to **Tools → Options → Graphical Mode → Diffusion**. Also see ["Global Settings: Diffusion Calculator" on page 45](#).



The Diffusion Module (DICTRA) in Console Mode has commands to perform some of the settings also available on the Diffusion Calculator. Where possible the name of the command is indicated and includes a link to the topic.

Simulation Conditions

Default solver

Automatic or Homogenization.

Select **Homogenization** to define additional sections.

ABOUT THE HOMOGENIZATION SOLVER

The homogenization solver (called the homogenization model in Console Mode) is useful when you want to simulate long-range diffusion through a multiphase mixture, under the assumption that local equilibrium holds at each node point.

TIME INTEGRATION METHOD**Automatic , Trapezoidal or Euler backwards.**

The default is **Automatic** where the default degree of implicitness corresponds to trapezoidal (0.5) for classic and Euler Backward (1.0) for the homogenization model. If large fluctuations occur in the profiles it may be necessary to use the more stable but less accurate *Euler backwards*.

SAVE RESULTS ON FILE

Yes, No or Every nth. . Select **Every nth** to enter a value in the field.

This setting is determine if the results are to be saved on file during the course of the simulation.

- **Yes** to always save on file
- **No** to never save on file
- **Every nth.** to save every n^{th} time to file. Then enter an integer value ranging from 0 to 99.

USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATIONS

The default **Automatic** allows the software program to automatically use forced starting values to perform the equilibrium calculations. When a phase with an ordering contribution is entered into the simulation, for example the gamma-prime/fcc_l12 phase in Ni-base superalloys, forced starting values are automatically turned on. Optionally choose **Yes** or **No**.

DEFAULT DRIVING FORCE FOR PHASES ALLOWED TO FORM AT INTERFACES

Enter a value in the field. The required driving force (evaluated as $DGM_{(ph)}$) to be used for

determining whether an inactive phase is stable. DGM is the variable for the driving force that is already divided by RT , and it is dimensionless. The default is $1E-5$.

► ["Suffixes" on page 390](#)

Timestep Control

MAX RELATIVE ERROR

Enter a value in the field. The default is 0.05.

MAX ABSOLUTE ERROR

Enter a value in the field. The default is $1.0E-5$.

TIMESTEP

Enter values in the fields.



This value is always in seconds.

- **Initial.** What is used as the initial time step. The default is $1.0E-7$.
- **Smallest allowed.** The smallest time step allowed during the simulation. This is required when using the automatic procedure to determine the time step. The default is $1.0E-7$.
- **Max % of simulation time.** The default is 10.

FACTOR SPECIFYING THE MAXIMUM INCREASE IN THE TIME STEP TAKEN FROM ONE TIME STEP TO ANOTHER

For example, if 2 is entered the maximum time step is twice as long as the previous time step taken.

Enter a value in the field. The default is 2.

THE TIMESTEP IS TO BE CONTROLLED BY THE PHASE INTERFACE DISPLACEMENT DURING THE SIMULATION

The default is **Automatic**. When a liquid phase is entered in a simulation this option is automatically turned on. Optionally choose **Yes** or **No** to set whether the time step is to be controlled by the phase interface displacement during the simulation.

Classic and Homogenization Model Settings

Classic Model Specific

ACTIVITY OR POTENTIAL

Use the [activity or potential] of a component in order to find the correct tieline at the phase interface.

Determines whether the program should use the potential or the activity of a component in order to find the correct tie-line at the phase interface. The potential or the activity is varied by the program and is set in order to reduce the degrees of freedom at the local equilibrium.

FLUX BALANCE EQUATION ACCURACY

Required accuracy during the solution of the flux balance equations. The default is $1.0\text{E}-16$.

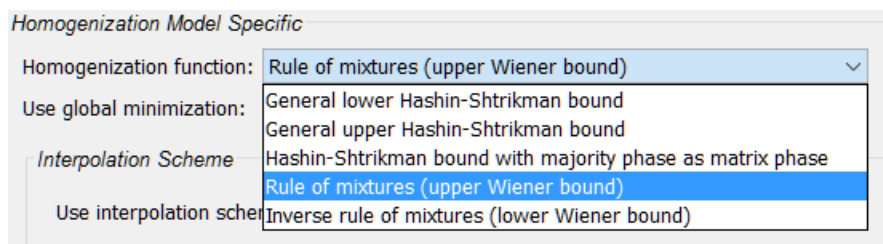
Homogenization Model Specific



This section is available when **Homogenization** is selected (or automatically selected) as the **Default solver**. These settings are available on the **Options** tab.

HOMOGENIZATION FUNCTION

Several functions are available. The default is **Rule of mixtures (upper Wiener bound)**. See ["About the Homogenization Functions" on the next page](#).



USE GLOBAL MINIMIZATION

Select the check box for global minimization used in equilibrium calculations. In general, using global minimization significantly increases the simulation time, but there is also a significantly reduced risk for non-converged equilibrium calculations.

INTERPOLATION SCHEME

When the homogenization model is used, simulations are run using an implicit finite volume method to increase numerical stability. Because of this, and other factors, homogenization model simulations generally run slower than other comparable simulations. You can reduce simulation time with the **Use Interpolation scheme** check box. The check box is selected by default.

DISCRETIZATION

[**Logarithmic** or **Linear**] discretization with *[number of]* steps in each dimension.

- For the linear discretization the scheme is not used at node points where the content of one or more solutes fall below a certain critical value. For such cases, where composition span many orders of magnitude, the logarithmic discretization can be tried.
- Enter the number of steps in composition space. In the limit where an infinite number of steps are used, exactly the same solution is obtained as without the interpolation scheme. However, excellent results can be obtained with a reasonable discretization. The default is 10000 steps.

MEMORY TO USE

This is the fraction of free physical memory to be used by the interpolation scheme.

Select **Megabyte** or **Fraction of free** and then enter a value in the field.

About the Homogenization Functions

The geometrical interpretation of the Hashin-Shtrikman bounds are concentric spherical shells of each phase. For the general lower Hashin-Shtrikman bound the outermost shell consists of the phase with the most sluggish kinetics and vice versa for the general upper bound. The geometrical interpretation of the Hashin-Shtrikman bounds suggest further varieties of the bounds, viz. *Hashin-Shtrikman bound with prescribed matrix phase* and *Hashin-Shtrikman bound with majority phase as matrix phase*, where the outermost shell consist of a prescribed phase or the phase with highest local volume fraction, respectively.

The geometrical interpretation of the Wiener bounds are continuous layers of each phase either parallel with (upper bound) or orthogonal to (lower bound) the direction of diffusion.



The labyrinth factor functions (described below) are only available in Console Mode.

The labyrinth factor functions implies that all diffusion takes place in a single continuous matrix phase. The impeding effect on diffusion by phases dispersed in the matrix phase is taken into account by multiplying the flux with either the volume fraction (*Labyrinth factor f with prescribed matrix phase*), or the volume fraction squared (*Labyrinth factor f^2 with prescribed matrix phase*), of the matrix phase.



The varieties with excluded phases (described below) are only available in Console Mode.

The varieties with excluded phases are useful in several respects. First, if a phase is modelled as having zero solubility for a component, the mobility of that component in that phase is undefined, which causes a (non-terminal) error. Setting a phase as excluded causes the mobility of all components in that phase to be set to zero. Second, often there are some major matrix solid solution phases and some minor precipitate phases. If the mobilities in the minor precipitate phases are zero the lower Hashin-Shtrikman bound is useless as it produces a kinetic coefficient of zero. However, using *General lower Hashin-Shtrikman bound with excluded phase(s)* the excluded phases are not considered when evaluating what phase has the most sluggish kinetics.

Pause, Resume and Cancel Diffusion Calculations

Diffusion calculations are often complex simulations that take some time to complete. Sometimes you may want or need to pause or resume a calculation, or make adjustments to your compositions and start again.

GRAPHICAL MODE

In Graphical mode, you pause and resume from the Diffusion Calculator **Configuration** window.

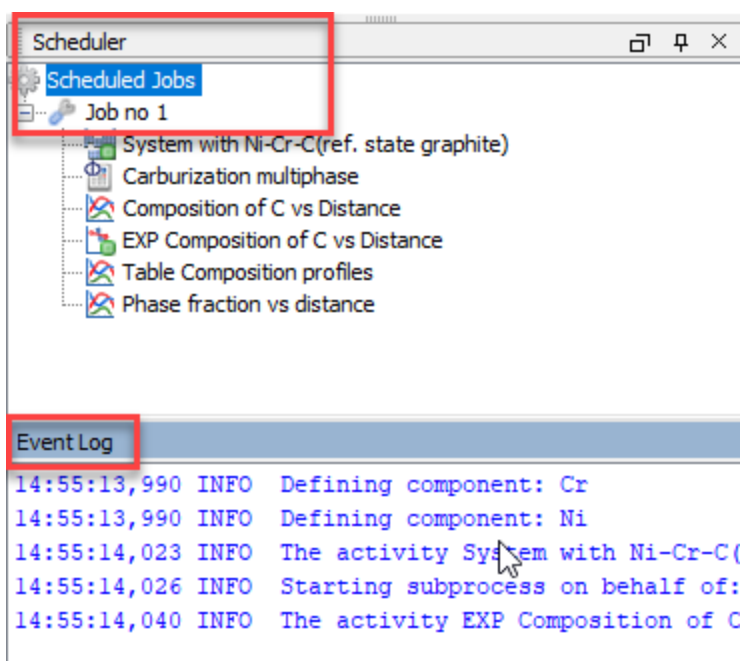


This is also available for the Precipitation Calculator (but not any other calculators). See ["Pause, Resume and Cancel Precipitation Calculations" on page 148](#).

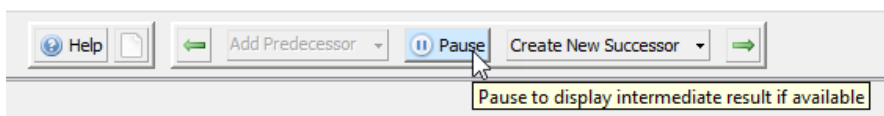
To Pause and Resume a Job

1. Run the job (i.e. click **Perform Tree**). In the **Scheduler**, you can see the job listed and

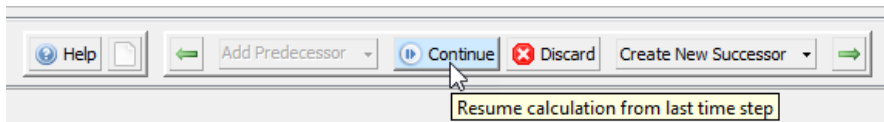
in the **Event Log** you can follow the progress of the calculation.



2. In the **Project** window, click the **Diffusion Calculator** node.
3. In the **Configuration** window at the bottom, click **Pause**. If there are intermediate results available these will be listed in the **Event Log**.

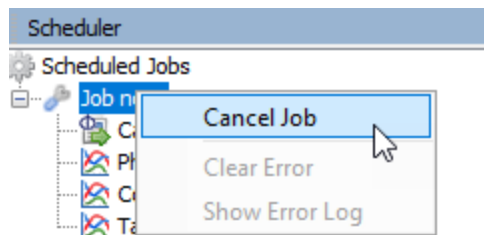


4. When ready, click **Continue** to resume your calculations from the last time step or click **Discard** to discard the calculation (then click **Yes** or **No** on the window that opens).



To Cancel a Job

- In the **Scheduler** window, right-click the job you want to cancel and select **Cancel Job**.



CONSOLE MODE

In response to a command or a lengthy calculation, Thermo-Calc may display a lot of text in the Console window. Use these keyboard shortcuts to pause, resume or stop a process.

- To pause the text on printing press <Ctrl+S>.
- To resume the printing on screen, press <Ctrl+Q>.
- When Thermo-Calc is performing a stepping or mapping operation, the results are continuously printed in the Console window. To stop the calculation of the current region of the mapping and stop the output, press <Ctrl-A> (Windows) or <Ctrl-C> (Linux).

Precipitation Calculator



The Precipitation Calculator is available with three elements if you do not have the additional Precipitation Module (TC-PRISMA) license. With the add-on module you can use all available elements. See ["Precipitation Module: Available Graphical Mode Features" below](#) for more information.

A Precipitation Calculator allows you to set the conditions for, and perform, a precipitation calculation. You can add the calculator to the System Definer directly (right-click and select it from the **Create New Successor** menu) or use the **Precipitation Simulation** template.

Once you have added a Precipitation Calculator, the **Configuration** window has these settings tabs:

- **Conditions:** Set the conditions for your calculation that define the Matrix and Precipitate phases. Choose the Calculation Type.
- **Options:** Modify Numerical Parameters that determine how the conditions are calculated. The Growth rate model can be set to Simplified or Advanced mode.

Precipitation Module: Available Graphical Mode Features

The Precipitation Module, previously referred to as TC-PRISMA, is an add-on module to the core Thermo-Calc software. A separate license is required to perform calculations for more than three elements. Without it you are able to use the module in *Demo Mode*.

► ["Demonstration \(Demo\) Mode" on page 131](#)

PRECIPITATION SIMULATION TEMPLATE

A **Precipitation Simulation** template is available to all Thermo-Calc users.

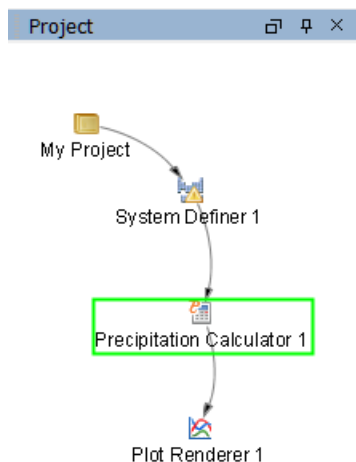


If you are accessing the Precipitation Module in Demo Mode, see ["Demonstration \(Demo\) Mode" on page 131](#) for what is available to you.

Using the Template

When you first open Thermo-Calc in Graphical Mode, on the **My Project** window, click the **Precipitation Simulation** button to add a *System Definer*, *Precipitation Calculator* and *Plot Renderer* to the **Project** tree.

Click the **Precipitation Simulation** button in the templates section to add these nodes to the Project.



▶ ["Creating a Project from a Template" on page 30](#)

PRECIPITATION CALCULATOR

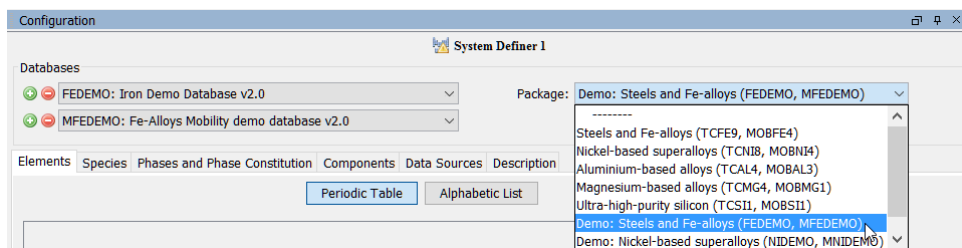
A Precipitation Calculator allows you to set the conditions for, and perform, a precipitation calculation.

DEMO DATABASE PACKAGES FOR THE EXAMPLES COLLECTION

Both a thermodynamic and mobility database are required to run the Precipitation Module simulation. If you have a Precipitation Module (TC-PRISMA) license you can run all the examples as the demonstration database packages are included with your installation. Select the database packages from the **System Definer**→**Configuration** window to run a simulation.



If you are using the Precipitation Module in Demo Mode, see ["Demonstration \(Demo\) Mode" on the next page](#) to learn more.



DEMONSTRATION (DEMO) MODE

The Precipitation Module, and some examples, are available to all Thermo-Calc users but only for simulations of alloys with up to three elements. If you do not have a license for the Precipitation Module then you are in *Demonstration Mode* when using the Precipitation Calculator or Precipitation Simulation template.

Precipitation Simulation Template

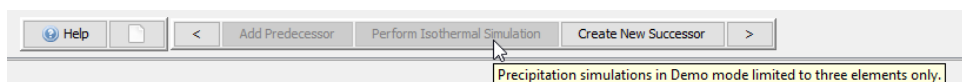
When you are in DEMO mode, in the **Templates** area this is indicated by the text under the logo.



Precipitation Calculator

If you are experimenting with the Precipitation Calculator in Demo Mode, you may have access to a variety of databases based on your license. However, you can only define up to three elements for a demo simulation.

If you define more than three elements on the System Definer, when you go to the Precipitation Calculator, the **Perform** button is unavailable and the tooltip explains why. In this case one of the chosen elements needs to be removed and then the Perform button is made available.





Even if you have more than three elements, the Plot Renderer or Table Renderer **Perform** button is still available. However, if you click the button and try to run the simulation the Event Log displays an error message.

Define the Precipitation Calculator

▶ ["Precipitation Module: Available Graphical Mode Features" on page 129](#)

Working with precipitation simulations is an advanced topic. It is recommended you review the Precipitation Module (TC-PRISMA) documentation and videos available or search for a specific topic.

1. Add a **Precipitation Calculator** node to the System Definer. If you used the **Precipitation Simulation** template, click the node to display the **Configuration** settings window.
2. In the Precipitation Calculator **Configuration** window, enter the settings described in ["Conditions Tab Settings" below](#). Additional advanced options settings are also available and described ["Option Tab Settings" on page 146](#).
3. Once you have finished defining the Precipitation Calculator, you also choose settings on the ["Plot Renderer" on page 179](#). Some additional settings are specific to the ["Plot Renderer" on page 189](#).

Conditions Tab Settings

Below are details about the settings available from the **Conditions** tab.

Configuration

Precipitation Calculator 1

Conditions Options

Composition unit: Mass percent

Composition Fe 99.984

Composition C 0.016

Matrix Phase

Phase: BCC_A2

▼ Show details

● Precipitate Phase

Phase: CEMENTITE

▲ Hide details

Nucleation sites: Dislocations ☒ Calculate from matrix settings 5.87951601467259E20 m⁻³

Interfacial energy: User-defined $f(r,T) = 0.24$ J/m²

Growth rate model: Advanced

Morphology: Sphere

Transformation strain: Disregard

Molar volume: Database 1.0E-5 m³/mol

Phase boundary mobility: 10.0 m⁴/Js

Phase energy addition: 0.0 J/mol

Approximate driving force: ☐

Preexisting size distribution: ☐ Edit particle size distribution

Calculation Type

☒ Isothermal ☐ Non-isothermal ☐ TTT diagram ☐ CCT Diagram

Temperature: 102.0 Celsius

Simulation time: 600000.0 Seconds

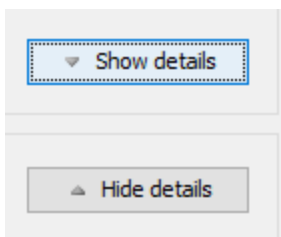
Help Add Predecessor Perform Isothermal Simulation Create New Successor



You can change these settings locally for a specific Precipitation Calculator or globally for some defaults in the **Options** settings. To open the Options window: From the main menu select **Tools** → **Options**. Click the **Graphical Mode** tab then click **Precipitation**.

Show or Hide Details

Click **Show details** (found to the right of the section) to view some of the additional settings listed below. You can also set the default to display in **Phase view mode** under **Tools → Options → Graphical Mode**, then click the **Precipitation** node.



Composition Unit

Choose from **Mass percent**, **Mole percent**, **Mass fraction** or **Mole fraction**.

Matrix Phase

Phase



Only phases with kinetic data can be selected as the matrix phase. If the list is empty, go to the System Definer to confirm that both thermodynamic and kinetic databases are selected and defined.

Choose a **Phase** from the list. The list is based on the settings for the System Definer. When setting up a system, choose a matrix phase with kinetic data available in the database.

Elastic properties

Choose **Disregard** to ignore the elastic properties.

Default elastic constants for **Isotropic** or **Cubic** are based on the major element of the alloy system. The elastic properties can affect nucleation rate, nuclei size, and particle shape.

- For **Isotropic**, enter values for **Shear modulus** (in GPa) and **Poisson's ratio** as required.
- For **Cubic**, enter values for **c11**, **c12** and **c44** as required. c_{11} , c_{12} , c_{44} are the elastic constants.

Molar volume

Use the **Database** value (if the molar volume for the phase is defined in the thermodynamic database) or select **User-defined** to enter another value.

Grain size

Grain size is the "diameter" of a grain. The **Grain size** value changes the available nucleation sites when **Grain boundaries**, **Grain edges**, or **Grain corners** is selected along with **Calculate from matrix settings** in the Precipitate Phase. Enter a numerical value and choose a unit from the list. The default is 1.0E-4 m.

Grain aspect ratio

For an elongated grain with a minor axis and a major axis, one may use the minor axis as grain size and the major/minor ratio as the grain aspect ratio to characterize the grain. The **Grain aspect ratio** value also changes the available nucleation sites when **Grain boundaries**, **Grain edges**, or **Grain corners** is selected along with **Calculate from matrix settings** in the Precipitate Phase. Enter a numerical value. The default is 1.0.

Dislocation density

The **Dislocation density** value changes the available nucleation sites when **Dislocations** is selected along with **Calculate from matrix settings** in the Precipitate Phase. Enter a numerical value. The default is 5.0E12 m⁻³.

Mobility enhancement prefactor

A parameter that multiplies to the mobility data from a database. This value scales the

mobility by a constant amount. This can be useful, for example, when the material has a higher than normal vacancy concentration at the start of the precipitation simulation. (e.g. from a prior solutionizing and quenching treatment).

Mobility enhancement activation energy

A value that adds to the activation energy of mobility data from a database. This value scales the mobility by a temperature dependent amount. Similar usage as mobility enhancement prefactor.

Precipitate Phase

Phase



The phases available to choose have both thermodynamic and kinetic data. If the list is empty, go to the System Definer to confirm that both types of databases are selected and defined.

Choose a **Phase** from the list. The list is based on the System Definer settings.

Nucleation sites

The number of different nucleation sites is dependent on the shape and size of grains in the matrix. Grain size is the "diameter" of a grain. Choose one of the following from the list.

- **Bulk, Grain boundaries, Grain edges, Grain corners, or Dislocations.**
- For **Grain boundaries, Grain edges** and **Grain corners**, enter the **Wetting angle (0-90)** in addition to the matrix settings. **Wetting angle** defines the deviation from spherical shape (or dihedral angle).

Click to select the **Calculate from matrix settings** check box if you want to calculate the number density of sites from the matrix grain size or dislocation density.

To enter a specific value for the number of **Nucleation sites**, deselect the check box.

Interfacial energy

Choose **Calculated** to use the estimated value. To adjust the estimate, enter a different **prefactor** or choose **User-defined** to enter a value in J/m². For the User-defined option, you

can also enter it as a function of radius (r) and temperature (T).

Growth rate model

Select **Simplified**, **General**, **Advanced**, **Paraeq** or **NPLE**. All models treat a particle (precipitate) of stoichiometric composition or with negligible atomic diffusivity. Local equilibrium or paraequilibrium at the precipitate-matrix interface is assumed.

Morphology

Choose the particle shape: **Sphere** (default), **Cuboid**, **Plate** or **Needle**. Options are based on the **Elastic properties** selected for the **Matrix** phase:

- For **Cubic**, **Sphere**, **Plate** , **Needle** and **Cuboid** are available.
- For **Isotropic**, **Sphere**, **Plate** and **Needle** are available.

For **Plate** or **Needle**, select the **Calculate aspect ratio from elastic energy** check box or enter a numerical value in the **Aspect ratio** field to provide a constant aspect ratio.

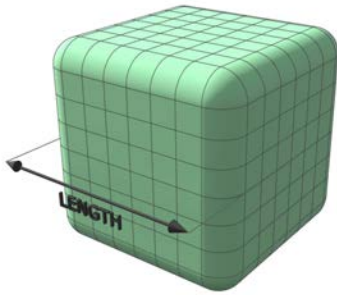


Figure 1: The cuboid shape is described by a supersphere. Cuboids have six faces, which form a convex polyhedron.

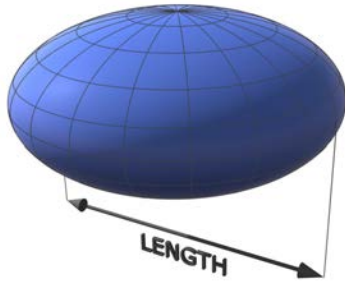


Figure 2: The plate is described as oblate spheroid. Oblate spheroids have rotational symmetry around an axis from pole to pole.

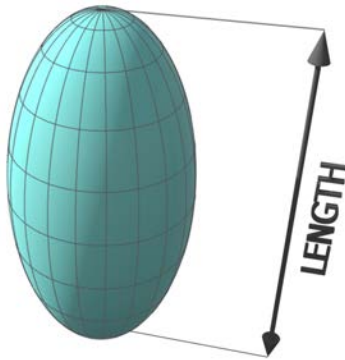


Figure 3: The needle shape is described as prolate spheroid. A prolate spheroid is a surface of revolution obtained by rotating an ellipse about its major axis.

Transformation strain

Choose **Disregard** to ignore the transformation strain. When **Isotropic** or **Cubic** is chosen in **Elastic properties** in Matrix Phase, you can also choose **Calculated from molar volume** to obtain a purely dilatational strain. If **Plate** or **Needle** is selected as the **Morphology**, you can alternatively choose **User-defined** and enter the properties for ϵ_{11} , ϵ_{12} , ϵ_{13} , ϵ_{22} , ϵ_{23} , and ϵ_{33} .

Molar volume

Use the **Database** value (if the phase molar volume is defined in the thermodynamic database) or select **User-defined** to enter another value.

Phase boundary mobility

A parameter that accounts for interface-controlled growth. Only effective if a very small, positive value is used. Use with caution due to a tentative treatment.

Phase energy addition

An energy value that adds to the Gibbs free energy of the precipitate phase from a database.

Approximate driving force

Select the check box to include this if simulations with several compositions sets of the same phase create problems.

Preexisting size distribution

Select the check box to include this. Click **Edit particle size distribution** to open the **Preexisting Particle Size Distribution** window where you can edit the parameters and view a graph comparing the radius and number density for the selected component.



Press F1 and search for "Particle Size Distribution (PSD)" for detailed instructions.



See examples [P_10](#) and [P_11](#)

Calculation Type

Isothermal

Use an **Isothermal** calculation type to do a precipitation simulation at constant temperature. Choose a unit of measurement and enter a numerical value for the **Temperature** and **Simulation time**.

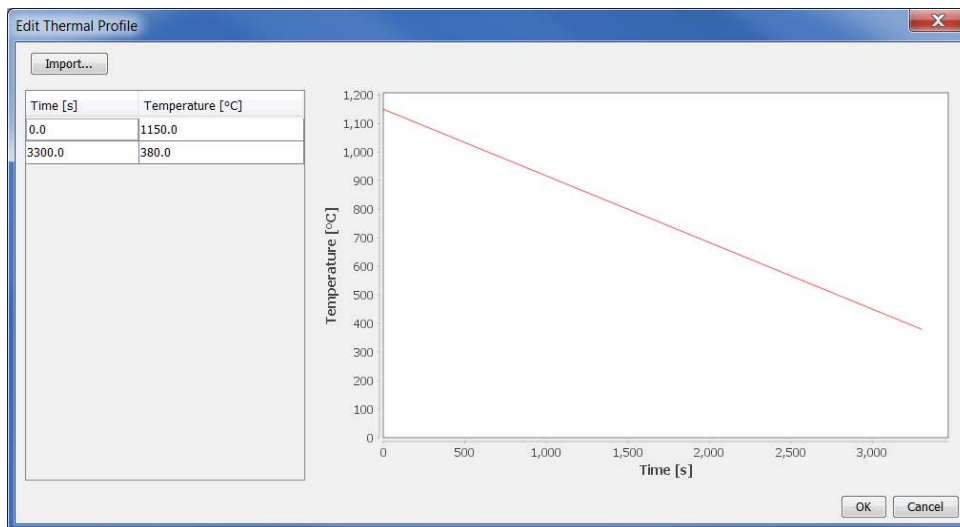


See examples [P_01](#), [P_02](#), [P_04](#), [P_05](#), [P_08](#) and [P_09](#)

Non-isothermal

Use a **Non-isothermal** calculation type to do a precipitation simulation with a user-defined temperature profile. Select a **Temperature unit** and **Time unit** from the lists. Enter a numerical value for the **Simulation time**.

Click **Edit thermal profile** to enter thermal profile **Temperature** and **Time** coordinates into a table. A minimum of two points is required. You can also **Import** to add your own **Thermal profile** from a text file in ***.xls**, ***.xlsx**, or ***.csv** formats.



See example [P_06](#)

TTT diagram

Use a **TTT-diagram** to calculate the time-temperature-transformation (TTT) curve for the formation of the precipitate phase.

- **Temperature:** Enter **Min**, **Max**, and **Step** numerical values and choose a temperature **Unit**.
- **Max annealing time:** Enter a numerical value and choose a time **Unit**.
- **Stop criteria:** Choose **Volume fraction of phase** or **% of equilibrium fraction** and then enter a numerical value. For each temperature, the simulation stops when the stop criteria is fulfilled or if the maximum annealing time is reached, whichever happens first.



See example [P_03](#).

CCT diagram

Use a **CCT-diagram** to calculate the continuous-cooling-transformation (CCT) curve for precipitation.

- **Temperature:** Enter **Min** and **Max** numerical values and choose a temperature **Unit**.
- **Cooling rate(s):** Enter a range of values in the field, e.g. .01 .1 1 10 100. These values are equal to **K/s**, **°C/s** or **°F/s** per second based on the temperature **Unit** selected.
- **Stop criteria:** Enter a numerical value for the **Volume fraction of phase**. For each temperature, the simulation stops when the stop criteria is fulfilled.



See example [P_07](#).

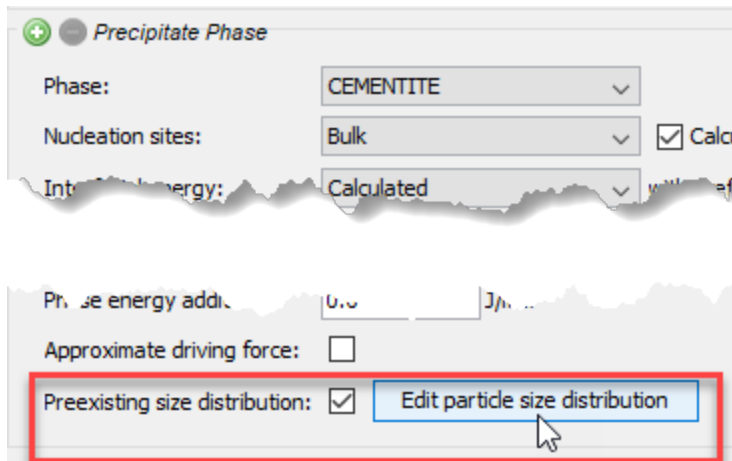
Particle Size Distribution (PSD)

On the Precipitation Calculator you can set the pre-existing particle size distribution (PSD) parameters in the **Show details** section. The size distribution can be entered as a pre-defined distribution, by importing a file, or by manually entering information into a table.

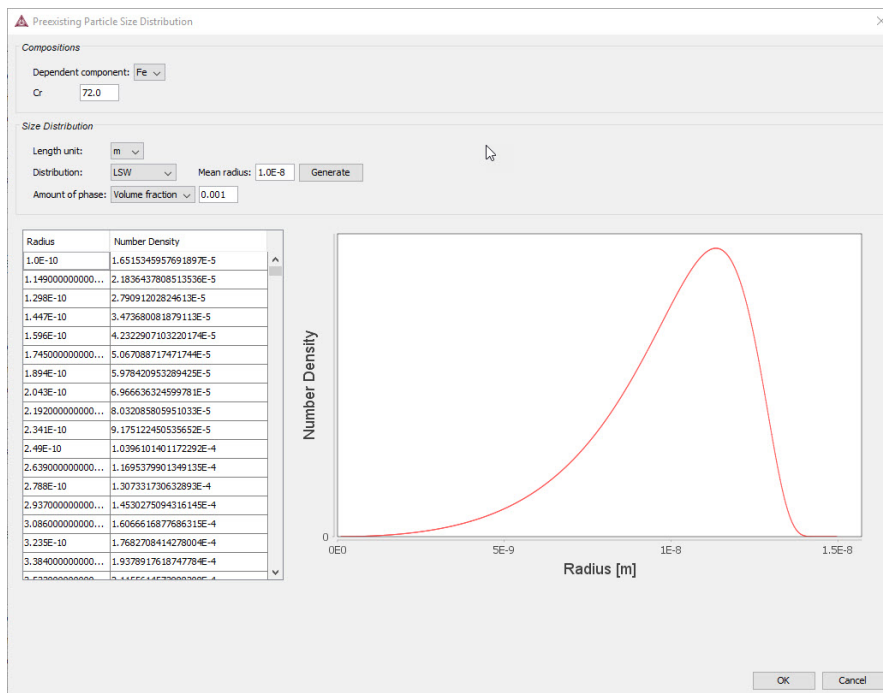
Accessing the 'Pre-existing size distribution' settings

1. To the right of the **Precipitate Phase** settings fields, click **Show details**.

2. Click to select the **Preexisting size distribution** check box.



3. Click **Edit particle size distribution** to open the window as in example P_10.

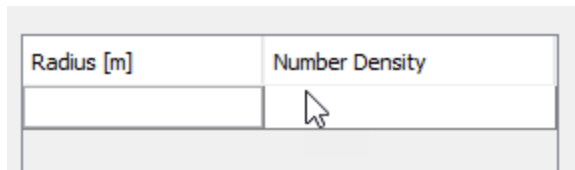


Defining the Preexisting size distribution

1. Under **Compositions**, choose a **Dependent component** from the list and enter the composition for the other component.

2. Under **Size Distribution** define the following:

- a. Choose a **Length unit**: m, μm , or nm.
- b. Choose a **Distribution**: **LSW** (Lifshitz-Slyozov-Wagner), **Normal**, **Log normal** or **From file**. You can also manually enter numbers into the table instead of importing a file.



| Radius [m] | Number Density |
|------------|----------------|
| | |
| | |

- c. For **LSW**, **Normal** and **Log normal**, enter a **Mean radius**.
- d. For **Normal** and **Log normal**, enter a value for the standard deviation (**Std**).
- e. For **From File**, click **Import** and navigate to the file containing the required information and click **Open**. This file can be in .xls, .xlsx, .csv or .txt formats. The file should consist of two columns with values where the first column contains **radius** data and the second contains **number density** data.
- f. For all options, choose an **Amount of phase**: **Volume percent** or **Volume fraction** and then enter a number in the field.
- g. Once the **Distribution** is defined, click **Generate**.

Option Tab Settings

These settings are for the Precipitation Calculator and are located on the **Configuration** window → **Options** tab.



You can change these settings locally for a specific Precipitation Calculator or globally in the **Options** settings. To open the Options window: From the main menu select **Tools** → **Options**. Click the **Graphical Mode** tab then click **Precipitation**.

Numerical Parameters

Click **Options** to go to these settings.

Max time step fraction

The maximum time step allowed for time integration as fraction of the simulation time. The default is 0.1.

No. of grid points over one order of magnitude in radius

Default number of grid points for every order of magnitude in size space. The default is 150.0.

Max no. of grid points over one order of magnitude in radius

The maximum allowed number of grid points in size space. The default is 200.0.

Min no. of grid points over one order of magnitude in radius

The minimum allowed number of grid points in size space. The default is 100.0.

Max relative volume fraction of subcritical particles allowed to dissolve in one time step

The portion of the volume fraction that can be ignored when determining the time step. The default is 0.01.

Max relative radius change

The maximum value allowed for relative radius change in one time step. The default is 0.01.

Relative radius change for avoiding class collision

Set a limit on the time step. The default is 0.5.

Max overall volume change

This defines the maximum absolute (not ratio) change of the volume fraction allowed during one time step. The default is 0.001.

Max relative change of nucleation rate in logarithmic scale

This parameter ensures accuracy for the evolution of effective nucleation rate. The default is 0.5.

Max relative change of critical radius

Used to place a constraint on how fast the critical radius can vary, and thus put a limit on time step. The default is 0.1.

Min radius for a nucleus to be considered as a particle

The cut-off lower limit of precipitate radius. The default is 5.0E-10 m.

Max time step during heating stages

The upper limit of the time step that has been enforced in the heating stages. The default is 1.0 s.

Maximum relative solute composition change at each time step

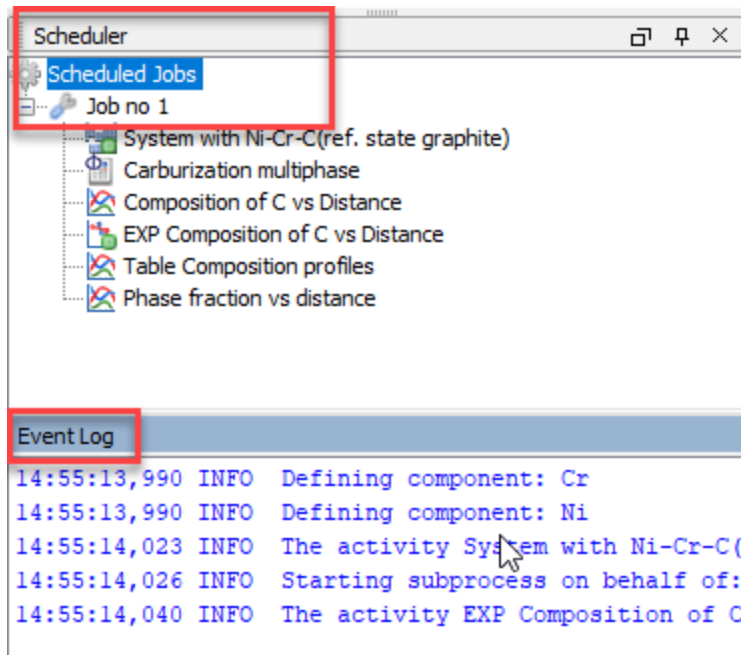
Set a limit on the time step by controlling solute depletion or saturation, especially at the isothermal stage. The default is 0.01.

Pause, Resume and Cancel Precipitation Calculations

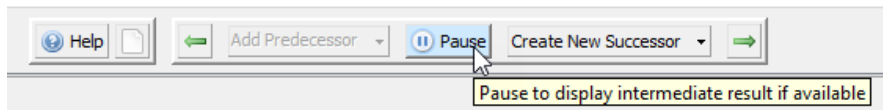
Precipitation calculations are often complex simulations that take some time to complete. Sometimes you may want or need to pause or resume a calculation, or make adjustments to your compositions and start again. You pause and resume from the Precipitation Calculator **Configuration** window.

To Pause and Resume a Job

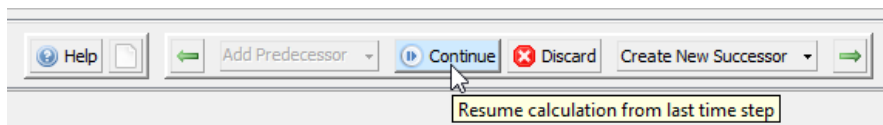
1. Run the job (i.e. click **Perform Tree**). In the **Scheduler**, you can see the job listed and in the **Event Log** you can follow the progress of the calculation.



2. In the **Project** window, click the **Precipitation Calculator** node.
3. In the **Configuration** window at the bottom, click **Pause**. If there are intermediate results available these will be listed in the **Event Log**.

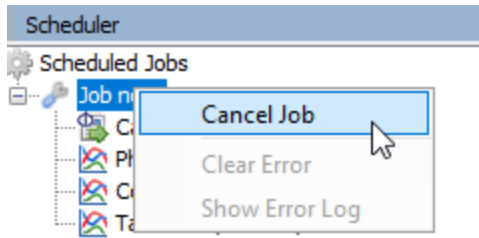


4. When ready, click **Continue** to resume your calculations from the last time step or click **Discard** to discard the calculation (then click **Yes** or **No** on the window that opens).



To Cancel a Job

- In the **Scheduler** window, right-click the job you want to cancel and select **Cancel Job**.



About the Process Metallurgy Module



The Process Metallurgy Module works with TCOX8 and newer versions of the database. The current version of the database is TCOX9.



All other users can test the module with the included OXDEMO database, which is limited to these elements: Al, C, Ca, Fe, O, S, and Si. For more information about this and other products [visit our website](#).

The Process Metallurgy Module is an add-on module to Thermo-Calc and it is available in Graphical Mode as the *Process Metallurgy Calculator*. The module is designed to model reactions that occur in metallurgical processes. It is based on the global equilibrium of the process. Although primarily used in steelmaking and steel refining processes (such as basic oxygen furnaces, electric arc furnaces, ladle furnace metallurgy and so forth), applications are not limited to steelmaking. The main difference compared to the a standard Equilibrium Calculator is that it is easy to handle the different materials present in a metallurgical process. The is especially true for the slag composition that is based on components.

Both isothermal and adiabatic calculations are possible. Adiabatic calculations assume no heat and mass exchange with the environment during the equilibrium reaction.

You can use the Process Metallurgy Module to calculate:

- The equilibrium between predefined steels and slags
- Desulfurization, dephosphorization, decarburization
- Any partition coefficient
- Slag characteristics, such as slag basicity or sulphur capacity
- The fraction of liquid and solid in the slag
- The temperature change in an adiabatic process

The module requires both a valid Maintenance and Support Subscription (M&SS) and a license for the TCS Metal Oxide Solutions Database (TCOX).

The Process Metallurgy Calculator

The materials are defined using the **Process Metallurgy Calculator**, which makes it easy to define the system by automatically including the three common material groups—*Steel*, *Slag* and *Gas*. The calculator has the default composition input types that are relevant to each material group. You can also save your material compositions right from the calculator and quickly access them in the future. For example, you might want to predefine compositions of steels, ferro-alloys, slags, and slag additions. The overall composition of the steel and slag is then obtained by adding amounts of these predefined materials.

Each group of materials is automatically added to the similar group where it is defined. You can manage these groups using the *Material Manager* (see ["Working with the Material Manager" on page 176](#)).

The calculations you can do with the module are *Single equilibrium*, *One axis*, *Grid* and *Uncertainty*. After adding a **Plot Renderer** or **Table Renderer**, you can choose a variety of quantities, including slag properties such as Bells ratio and B2, to output results that provide useful visual representations of the steelmaking systems you are analyzing.



["Process Metallurgy Calculator" on page 163](#) and ["Defining the Process Metallurgy Calculator" on page 164](#)



There are example project files included with the module and these examples are also explained in video tutorials available on our website and YouTube channel. For more information see ["PMET_01: Basic Oxygen Furnace \(BOF\)" on page 288](#), ["PMET_02: Ladle Furnace" on page 294](#) and ["PMET_03: Argon Oxygen Decarburization" on page 301](#).

Working with the Process Metallurgy Module

Working with the **Process Metallurgy Calculator** allows you to easily define complex metallurgical reactions. The calculator streamlines how you set up these steel and slag systems but there are details about various inputs and outputs that are different from other calculators. This topic is a general collection of information related to the Process Metallurgy Module and is intended to help you better understand how to interpret and make choices when you are setting up your steelmaking simulation.



Several internal calculations of the Process Metallurgy Module (for example for the determination of the component compositions of ionic phases) have a tight dependency on the database being applied. Therefore, it is only possible to use the module with the databases TCOX8, TCOX9 and OXDEMO. It is not possible to use custom user databases.

Working with Material Groups (Steel, Slag and Gas)

- ▶ For more details about these fields, see ["Defining the Process Metallurgy Calculator" on page 164.](#)
- ▶ For information about saving and deleting materials, see ["Working with the Material Manager" on page 176.](#)

There are three groups to define: **Steel** (or another user-defined **Metal** group), **Slag** and **Gas**.

In the image below, the red-highlighted area is where the Steel material group is defined. The drop-down menu that displays *Steel_BOF* shows a user-defined material. This can be defined and then saved to the material library.

When you click **Show composition** next to any material group, additional fields display for giving composition and input type where you can further define each material group. You can remove materials and add and remove material groups using the Material Manager (available via the **Tools** → **Options** menu).

After opening the ["PMET_01: Basic Oxygen Furnace \(BOF\)" on page 288](#) example, click **Show composition** next to the **Slag** and **Gas** groups to see how the *Slag_BOF* and *Oxygen* materials are defined.



You can open the example project file from Thermo-Calc **Help** → **Example Files** → **Process Metallurgy** → **PMET_01_Basic_Oxygen_Furnace.tcu**.

From this composition area you can click the **Save material** button to add the new material to the group's list. The newly named material composition is then available for use with that material group. In this example, the *Steel_BOF* material was defined first and then named at the end. It is now available in the lists wherever you select the Steel material or need to choose quantities to plot.

Configuration

Process Metallurgy Calculator 1

Conditions Options

Database: OXDEMO

Thermal control: Isothermal

Temperature: Celsius 1650.0

Pressure: Pascal 100000.0

Material: Steel Steel_BOF

Amount: Tonne 100.0 Hide composition

Input type: Mass percent Element Major component Save material

Major component: Fe 94.5

C 4.5

Si 1.0

Total: 100.0

Material: Slag Slag_BOF

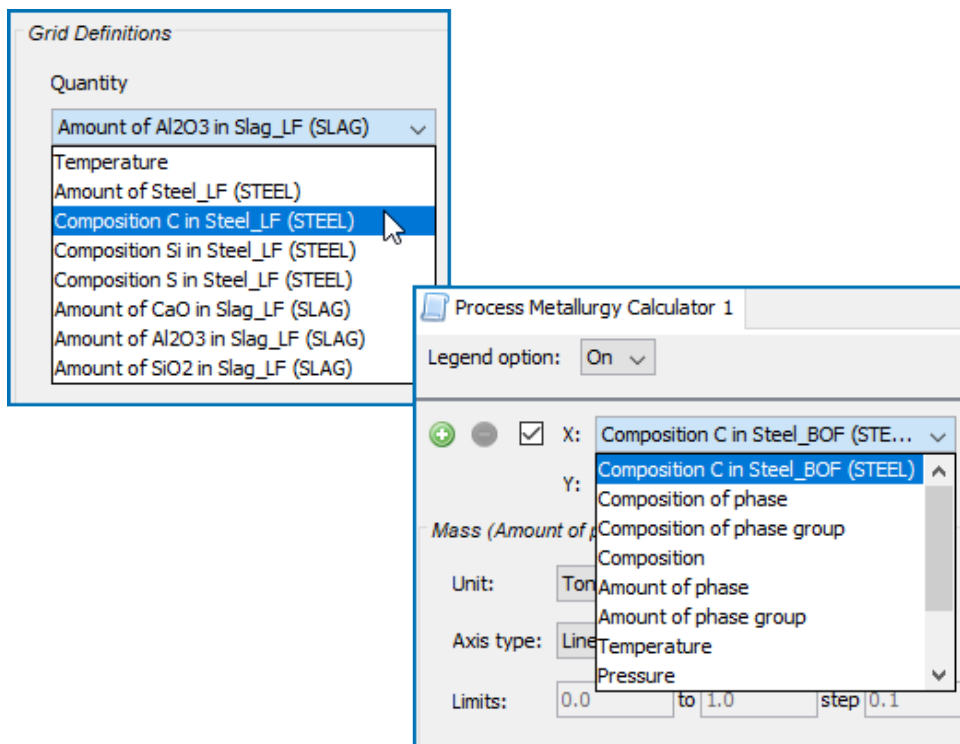
Amount: Tonne 3.0 Show composition

Material: Gas Oxygen

Amount: Normal cubic meter 0.0 Show composition

Calculation Type

The three material group areas on the Process Metallurgy Calculator where you can define components and save materials. You can create your own material groups using the Material Manager.



After defining and saving a material composition, the named material is available for selection in a variety of places such as when choosing quantities on the calculator and defining axis variables on the Plot Renderer.



To add one or more material groups click the green add button. Click the red minus button to remove a material group. The new material inherits the default settings of that group.

Understanding the Grid Definitions Quantities and How These Relate to the Composition

When you choose a **One axis** or **Grid Calculation Type**, you also choose a **Quantity** under the *Grid Definitions*. The relationship between these quantities and how the material group composition is defined is as follows.

The following uses **Composition of C in Steel_LF (STEEL)** as an example quantity for a **One axis** calculation.

Under *Grid Definitions*, the availability of the **Quantity** in the list is based on the material (**Steel_BOF**) that is defined and saved for the **Steel** group (or any user-defined metal, slag or gas group).

The screenshot shows two panels from a software interface. The 'Conditions' panel on the left has a 'Database' dropdown set to 'OXDEMO', 'Thermal control' set to 'Isothermal', 'Temperature' set to 'Celsius' with a value of '1650.0', and 'Pressure' set to 'Pascal' with a value of '100000.0'. Below these, 'Material' is set to 'Steel' and 'Steel_BOF', 'Amount' is 'Tonne' with a value of '100.0', 'Input type' is 'Mass percent', and 'Major component' is 'Fe' with a value of '94.5'. The 'Grid Definitions' panel on the right shows a table with columns 'Quantity', 'Min', 'Max', and 'Number of steps'. The first row is 'Temperature' with values 1500.0, 2000.0, and 10. The second row is 'Composition C in Steel_BOF (STEEL) [Mass percent]' with values 0.0, 1.0, and 10.

Defining the Material Composition

When you choose the **Input type** for a steel the composition of the elements can be set up using a combination of settings starting with **Mass** or **Mole percent**, **Mass** or **Mole fraction** or **Absolute amount**. Then you further choose to define the composition using either the **Major component** or **Normalize to total of 100%** options.



The *Amount of X in Y* quantities you can choose from the various drop-down lists (such as under *Grid Definitions*) are defined as Min-Max variation of the component X in Y. If a dependent element is present that is adapted as usual.

The screenshot shows two dropdown menus. The first dropdown, labeled 'Input type:', is open and shows a list of options: 'Mass percent', 'Mass fraction', 'Mole percent', 'Mole fraction', and 'Absolute amount'. The second dropdown, labeled 'Major component:', is also open and shows a list of options: 'Major component', 'Normalize to total of 100%', and 'Major component'.

When you use **Major component**, as you add other components or adjust the composition, the major one is adjusted to be the rest of the composition.

Major component:

+

-

Fe

94.5

+

-

C

4.5

+

-

Si

1.0

Total: 100.0

Major component:

+

-

Fe

93.5

+

-

C

5.5

+

-

Si

1.0

Total: 100.0

When you use **Normalize to total of 100%**, the sum is adapted to 100%. This is useful if you need to work with a given composition that does not sum up to 100%.

+

-

Fe

93.5

94.4444

+

-

C

4.5

4.54545

+

-

Si

1.0

1.01010

Total: 99.0 100.0

+

-

Fe

93.5

93.5

+

-

C

5.5

5.5

+

-

Si

1.0

1.0

Total: 100.0 100.0

Sometimes its preferable to use input of amount of each component **Amount** by weight (**Tonne, Kilogram, Gram** or **Pound**), it can useful to choose **Absolute amount** as the **Input type**. In this case, the total amount of material automatically adjusts the total.

| | | |
|-------------|-----------------|-------------|
| Material: | Steel | Steel_BOF |
| Amount: | Tonne | 100.0 |
| Input type: | Absolute amount | Element |
| | Fe | 94.5 94.5 |
| | C | 4.5 4.5 |
| | Si | 1.0 1.0 |
| Total: | | 100.0 100.0 |

| | | |
|-------------|-----------------|---------------|
| Amount: | Tonne | 101.0 |
| Input type: | Absolute amount | Element |
| | Fe | 94.5 93.5643 |
| | C | 5.5 5.44554 |
| | Si | 1.0 0.99009 |
| Total: | | 101.0 100.000 |

For the Gas component, if you choose **Normal cubic meter** as the **Amount**, then beside regular mass units, the amount of gas can also be provided in Nm³.

Configuration

Argon Oxygen Decarburization - calculator

Conditions Options

Database: TCOX9

Thermal control: Adiabatic

Temperature: Celsius

Pressure: Pascal 100000.0

Material: Steel Steel scrap with temperature: 1550.0

Amount: Tonne 40.0 Show composition

Material: Steel Ferrochrome with temperature: 20.0

Amount: Tonne 6.0 Show composition

Material: Gas Ar-O2 gas with temperature: 20.0

Amount: Normal cubic meter 1000.0 Show composition

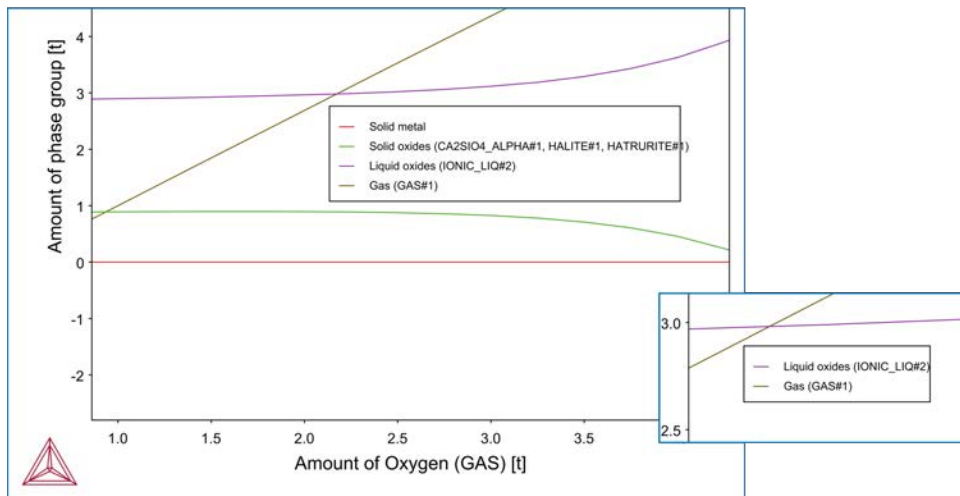
Phase Groups

The phases that are plotted after you run a simulation are grouped together on the plot to make the interpretation of the results easier.

Phases of similar type are bundled together in the groups *liquid metal*, *solid metal*, *solid oxides*, *liquid oxides* and *gas*. Except for the gas phase, all the groups can have more than one phase. This grouping is particularly useful for liquid metal and liquid oxide because they are both described by the same phase, IONIQ_LIQUID, and because there is typically two or more compositions sets of IONIQ_LIQUID. This is also useful for solid oxides, because a large number of phases can be stable, making the interpretation of results difficult without this grouping.



The term *oxides* in the Process Metallurgy Module can also mean carbides, sulfides and fluorides.



Example of the plot labels with the phases grouped together. As you zoom in, only the phases that you can see are listed in the label, making it easier to examine the results.

Slag Property Quantities

The slag properties are describing the capability of a slag to take up sulphur from the metal melt. The Process Metallurgy Module defines so-called phase groups. They contain all phases of a certain kind, for example all solid slag or all slag phases. The component composition of such a phase group is calculated by weighting the component composition of each phase with their fraction in the group.

This allows to calculate slag properties for the phase groups, for example for the overall slag.

On the Plot Renderer (for axis quantities) and Table Renderer there is an option to choose or define the **Slag property**. The associated quantity that you select has these options: **All**, **B2**, **B3**, **B4**, **Bas2**, **Bells ratio**, **Ls** , or **Log10 (Sulphur capacity)**.

- Details, including references and equations, are described in ["Process Metallurgy Slag Properties" on the next page](#).

Adiabatic Calculations

When setting up the Process Metallurgy Calculator you choose the thermal control to be either **Isothermal** or **Adiabatic**. Adiabatic calculations assume no heat and mass exchange with the environment during the equilibrium reaction. The adiabatic process is implemented by an isenthalpic process with constant pressure (i.e. $H=\text{const}$), which is equivalent.

- ["Adiabatic Calculations: Calculation of the Material Enthalpy" on page 162](#)

Gas Volume Units

Beside regular mass units, the amount of gas can also be provided in Normal cubic meter (Nm^3). The applied reference conditions are 1013.25 hPa and 15.0 °C (according to ISO 2533).



There are slightly deviating definitions present in the industry, which need to be converted for precise results. For most applications of the Process Metallurgy Module this difference has a minor influence.

Calculation of Component Compositions

The composition of all ionic phases is provided as elemental as well as component composition (i.e. Fe_2O_3 , FeO , CaO , ...). In order to provide a representation similar to that usually used in the industry, the content of S is provided as elemental content and the content of P is given as component content of P_2O_5 . This is a simplification because P and S can also be present as sulphates and phosphates in the slag and can bind to different metal cations. This can cause deviations in the overall component composition if the content of S and P is high in the phases. In doubt, the elemental composition can be used, it will always be exactly correct.

For non-ionic phases such as ALABANDITE, always the elemental composition will be shown only. This is also true if the IONIC_LIQ composition cannot be described by components only due to constraints of the overall composition (for example if the material has been oxidized completely and forces a certain composition of the ionic liquid slag).

Definition of Partial Pressure of Oxygen

The oxygen partial pressure in the gas phase is calculated with the following formula:

$$p_{O_2} = p \cdot AC(O_2, GAS)$$

In the formula, p describes the total system pressure and AC the activity of oxygen in the gas phase.

Activities of Slag Components

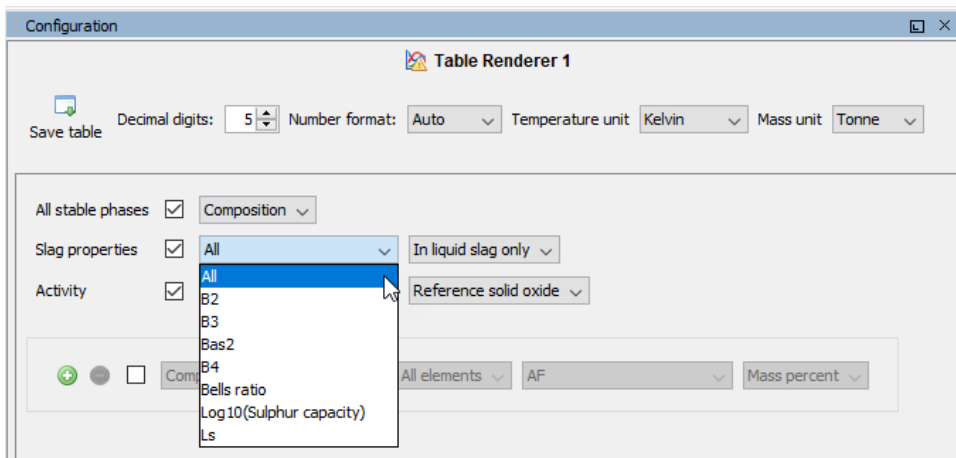
The chemical activity of each component $AC(COMPONENT, REFERENCE_PHASE)$ is available either with reference to the liquid or the solid slag phase. It can only be calculated for components being present in the thermodynamic database.

Process Metallurgy Slag Properties

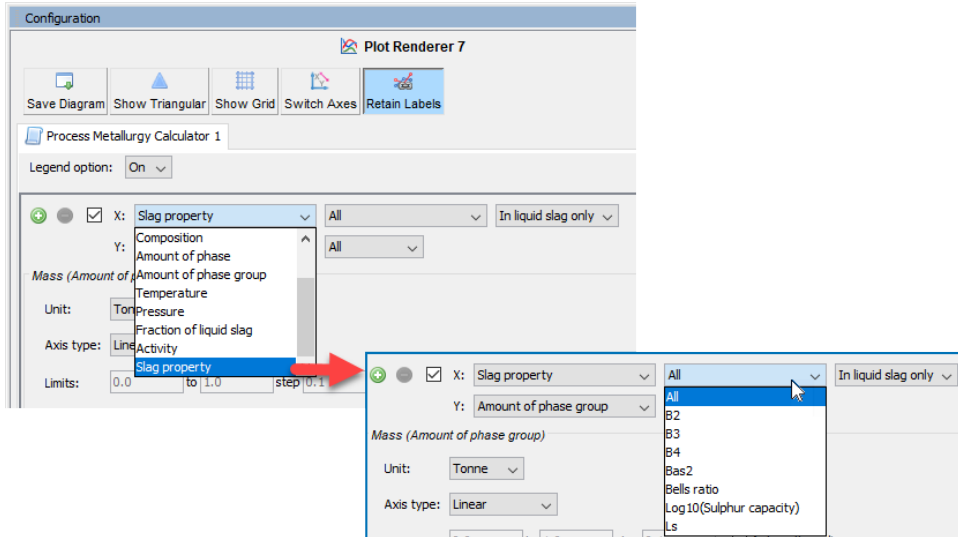
The slag properties are describing the capability of a slag to take up sulphur from the metal melt. The Process Metallurgy Module defines so-called phase groups. They contain all phases of a certain kind, for example all solid slag or all slag phases. The component composition of such a phase group is calculated by weighting the component composition of each phase with their fraction in the group.

This allows to calculate slag properties for the phase groups, for example for the overall slag.

For the **Process Metallurgy Calculator** when you are selecting axis variables on the **Plot Renderer** or choosing the properties to list with the **Table Renderer**, there is an option to include the slag properties. The associated quantity that you select from the next drop-down list has these options to choose: **All**, **B2**, **B3**, **B4**, **Bas2**, **Bells ratio**, **Ls**, or **Log10(Sulphur capacity)**. Also choose **In liquid slag only**, **In solid slag only** or **In all slag**. Depending on this setting, the composition averaged over liquid, solid or all slag is applied as a basis for the slag property calculation.



Slag properties for a Table Renderer



Slag properties for a Plot Renderer

Equations and References

The equations and references for these quantities are defined below. Composition can be given in mass (%) or fraction).

The formulas are given in Thermo-Calc console-like syntax (B: mass, W: weight fraction, AC: activity). A slag property will be available if all of its components are present in the phase group. Steel and slag are the actual phase groups chosen depending on the user request, i.e. the slag property can be calculated for the liquid slag only or for the overall slag (liquid and solid).

Basicity is defined as:

$$B2 = \frac{B(CaO)}{B(SiO_2)}$$

$$B3 = \frac{B(CaO) + B(MgO)}{B(SiO_2)}$$

$$B4 = \frac{B(CaO) + B(MgO)}{B(SiO_2) + B(Al_2O_3)}$$

$$Bas2 = \frac{B(CaO) + B(MgO)}{B(SiO_2) + B(Al_2O_3) + B(TiO_2)}$$

$$Bells\ ratio = \frac{B(CaO) + 0.7 \cdot B(MgO)}{0.94 \cdot B(SiO_2) + 0.18 \cdot B(Al_2O_3)}$$

Sulfur capacity is defined as:

$$L_s = \frac{W_{(slag)}(S)}{W_{(slag)}(S)}$$

$$\text{Log}_{10}(C_s) = \lg(W_{(slag)}(S) \cdot 100 \cdot \left(\frac{AC(O_2, GAS)}{AC(S_2, GAS)}\right)^{(0.5)})$$

REFERENCES

- **Basicity and MgO Saturation:** For definitions of the basicity and MgO saturation properties B2, B3, B4 and Bells ratio see Keskitalo (2015). Also see the Slag Atlas (Verein Deutscher Eisenhüttenleute, 1995).
- **Sulfur Distribution and Capacity:** For definitions of the sulfur distribution properties L_s see Andersson et al (1999). For the sulfur capacity, see Slag Atlas (Verein Deutscher Eisenhüttenleute, 1995).

Andersson, Margareta A. T., Par G. Jönsson, and Mselly M. Nzotta. 1999. "Application Ladle Slags of the Used Sulphide Capacity Concept on High-Basicity in Bearing-Steel Production." *ISIJ International* 39 (11): 1140–49.

Keskitalo, Björn. 2015. "Model Studies on the Effects of Composition Differences of Direct Reduction Pellets and an Adaptive Addition of Slag Formers for the EAF Process." Master's thesis, KTH Royal Institute of Technology, <http://urn.kb.se/resolve?urn=urn:nbn:se:kth:diva-168296>.

Verein Deutscher Eisenhüttenleute (VDEh), ed. 1995. *Slag Atlas* 2nd Edition. Dusseldorf, Germany: Verlag Stahleisen GmbH.

Adiabatic Calculations: Calculation of the Material Enthalpy

An adiabatic calculation requires the enthalpy of the input materials as an initial condition. The Process Metallurgy Module uses different approaches for the different material types metal, gas and slag.

METAL

Frozen-in global equilibrium calculation at $T=700\text{ °C}$, taking the resulting enthalpy at the actual initial material temperature. This corresponds to a frozen-in microstructure. At initial material temperatures above 700 °C the equilibrium is instead calculated directly.

GAS

Mechanical mixture between the enthalpy of the gas components. This is no limitation,

because all gas components in the database are assumed to be ideal gas.

SLAG

- **Mechanical mixture:** If the temperature is below $T=1000\text{ }^{\circ}\text{C}$ and every single material component (such as MgO , CaO , ...) is fully solid at the requested material temperature, mechanical mixture is assumed. This means that the enthalpy of every component is calculated separately and summed up (weighted by mass fraction). This corresponds to the assumption that different separate components have been added to the slag (such as burnt lime and magnesite). If any component forms gas or liquid at the initial material temperature, this mode is not used. Note that mechanical mixture is also applied if pure elements are added to the slag material, i.e. it is not the same in respect to the material enthalpy to define CaO and $\text{Ca} + \text{O}$.
- **Equilibrium:** If no mechanical mixture of the material components is possible or if the temperature is above $T=1000\text{ }^{\circ}\text{C}$. This corresponds to the assumption of a fully homogenized slag material.

Process Metallurgy Calculator

- For information about licenses and availability, see ["About the Process Metallurgy Module" on page 150](#).

Use a **Process Metallurgy Calculator** to set up calculations for steel and slag used in steel making. Define the composition of a steel (or other metal) and slag system using material groups: one each for steel, slag and gas. You can save your material compositions right from the calculator and quickly access and manage the materials and groups—it collects groups of saved materials according to type, thus making it easy to retrieve them.

You can add the calculator to **My Project** directly (right-click and select it from the **Create New Activity** menu) or use the available ["Process Metallurgy Template" on page 32](#).



Your installation includes examples that you can run to see how the calculator works. For more information see ["PMET_01: Basic Oxygen Furnace \(BOF\)" on page 288](#), ["PMET_02: Ladle Furnace" on page 294](#) and ["PMET_03: Argon Oxygen Decarburization" on page 301](#).

Conditions and Options Tabs

Once you have added a Process Metallurgy Calculator, the **Configuration** window has **Conditions** and **Options** settings tabs where you define the materials and choose the calculation type for the simulation.

CONDITIONS

Set the conditions for your calculation that define the slag, metal and gas. The topic, ["Defining the Process Metallurgy Calculator" below](#), has instructions that walk you through the steps that represent a simplified steelmaking process. For information about the individual settings on this tab, see ["Conditions Tab " on page 168](#).

OPTIONS

Modify some defaults related to process material equilibrium and grid settings such as step size, driving force and the minimization strategy.

► For information about the individual settings, see ["Options Tab " on page 174](#).

The **Options** tab is where you can locally define specific Process Metallurgy Calculator settings. These settings can also be applied globally from the **Options** window. From the Global options you can also manage the materials. See ["Working with the Material Manager" on page 176](#).



To open the **Options** window: From the main menu select **Tools → Options → Graphical Mode** and click the **Activities** tab. Then click **Process Metallurgy**. See ["Global Settings: Process Metallurgy " on page 45](#) for details.

Plots and Tables

Right-click the node to add a ["Plot Renderer" on page 179](#) or ["Table Renderer" on page 194](#) to visualize your results. Although both nodes work the same as with the other calculators in Thermo-Calc, there are a few extra features and settings unique to the Process Metallurgy Module. Useful information is included throughout the documentation. You can also read more about the unique features in ["Working with the Process Metallurgy Module" on page 151](#).

Defining the Process Metallurgy Calculator

After adding a **Process Metallurgy Calculator** to your project, you can define the steel, slag and gas groups of materials. The following is a general overview of the setup based on the ["PMET_01: Basic Oxygen Furnace \(BOF\)" on page 288](#) example, which walks you through the steps that represent a simplified steelmaking process.



See the Process Metallurgy Module examples that are available as video tutorials on our [website](#) and our [YouTube](#) channel.

Add the calculator, select a database and enter a temperature

-
1. Add a **Process Metallurgy Calculator** node to **My Projects** node. If you used the **Process Metallurgy** template, click the node to display the **Configuration** settings window.
 2. In the **Configuration** window, for the **Database** selection, the program automatically defaults to the highest version of the TCOX database (the current version is TCOX9), starting with TCOX8. For users without a license, the OXDEMO database is available and this allows for calculations using only these elements: Fe, C, S, Ca, Si, Al and O.
 3. Set the **Thermal Control** as being **Isothermal** or **Adiabatic**.
 4. Select a **Temperature** unit (**Kelvin**, **Celsius** or **Fahrenheit**) and enter a numerical value in the field.

Define the conditions for the steel, slag and gas material groups

Next you will define each material group—**Steel** (or any user-defined **Metal** group), **Slag** and **Gas**.

▶ See ["Conditions Tab " on page 168](#) for an overview of the layout of this section. There is also an overview of these material groups in ["Working with the Process Metallurgy Module" on page 151](#).



1. Choose a **Material** to set up first, **Steel** (or any user-defined metal), **Slag** or **Gas**.
2. Select an **Amount** from the list—**Tonne**, **Kilogram**, **Gram** or **Pound**. Enter a numerical value in the field.
3. To the right of the **Material** list (e.g. for the **Steel** group), choose the material composition you want to use for this simulation. Predefined **Example Steel** and **Example Slag** compositions are included with your installation.
 - If you chose **Adiabatic** as the **Thermal Control**, also enter a **temperature** in the field for each material. This is the initial temperature before the material is added to the process.
4. If this is the first time you are defining a material, or at any time when **User-defined** is selected, click **Show composition** to set the composition for the material (steel, slag or gas or another user-defined metal).



The composition for each material is hidden by default because the module allows you to easily save materials and access these from the material menu. Once you save a collection of materials, you will rarely have to click **Show composition**. See ["Working with the Material Manager" on page 176](#) for details about saving and deleting materials.

5. From the first **Input type** list select **Mass percent**, **Mass fraction**, **Mole percent**, **Mole fraction**, or **Absolute amount**. For **Absolute amount**, you can directly enter values in the fields in the unit selected above for Amount (**Tonne**, **Kilogram**, **Gram** or **Pound**).
6. For the next list, the default is based on which group you are defining. For the Steel (Metal) group it is **Element**, for Slag it is **Component** and for Gas it is **Gas component**.
7. Choose **Major component** so that as you add other components, the major one is adjusted to be the rest of the composition. Choose **Normalize to total of 100%** so that the sum is adapted to 100%. This is useful if you need to work with a given composition that does not sum up to 100% If you select **Absolute amount**, **Normalize to total of 100%** is not available.
8. Based on which material group you are working with, add the **Element**, **Component** or **Gas component**.



To add one or more material groups click the green add  button. Click the red minus  button to remove a material group. The new material inherits the default settings of that group.

9. After you have added and defined the element, component or gas component it is recommended you save and name the material. This makes it easier to work with because the name of the material is automatically updated in the lists (and available as part of your library) instead of being named *User-defined* everywhere.

The material is automatically saved in the relevant material group, so only steel materials are shown in the steel menu, only slag materials are shown in the slag menu and only gas in the gas menu. You can also create additional material groups if there are groups you use regularly, such as scrap compositions, ferro-alloys or slag additions. See ["Working with the Material Manager" on page 176](#) for more details about creating and deleting material groups and deleting materials.

- Continue adding and defining the material groups (e.g. Steel, Slag and Gas). You could, for example, add another Steel group if you wanted to define a composition of a steel scrap to add to a basic oxygen furnace (BOF).

Select the Calculation Type and associated definitions

► These settings are described more in ["Conditions Tab " on the next page](#).

- Under *Calculation Type*, click to choose **Single** (no axes), **One axis**, **Grid** or **Uncertainty**.



For more complex calculations, it is good practice to start with a **Single** equilibrium calculation to make sure the calculation converges. Also see the settings described in ["Options Tab " on page 174](#). These can be useful if your calculation fails.

- Based on the calculation type, define either the *Grid Definitions* (for **One axis** or **Grid** calculations) or the *Sampling of Data from Gaussian Distributions* (for **Uncertainty** calculations). The **Quantity** displays all the stepping options set up with the material groups for **Steel**, **Slag** and **Gas**. The example shows the steel group quantities.

Grid Definitions

| Quantity | Min | Max |
|---------------------------------------|-----|-----|
| Amount of Fe in Example Steel (STEEL) | 0.0 | 1.0 |
| Amount of Fe in Example Steel (STEEL) | | |
| Amount of C in Example Steel (STEEL) | | |
| Amount of Mn in Example Steel (STEEL) | | |
| Amount of P in Example Steel (STEEL) | | |
| Amount of S in Example Steel (STEEL) | | |
| Amount of Si in Example Steel (STEEL) | | |
| Amount of Al in Example Steel (STEEL) | | |
| Amount of O in Example Steel (STEEL) | | |

Select quantity for this axis



The *Amount of X in Y* quantities you can choose from the various drop-down lists (such as under *Grid Definitions*) are defined as Min-Max variation of the component X in Y. If a dependent element is present that is adapted as usual.



How these quantities relate to the material definition is described in ["Working with the Process Metallurgy Module" on page 151](#).

Add and define a plot or table and run the simulation

Once you have finished defining the Process Metallurgy Calculator, you also define the plot or table settings. To add a Plot Renderer or Table Renderer, right-click the calculator node and select an option from the **Create New Successor** menu.



The settings are generally described for the individual nodes. See ["Plot Renderer" on page 179](#) and ["Table Renderer" on page 194](#).



Some useful information about the plots is also described in ["Working with the Process Metallurgy Module" on page 151](#).

Conditions Tab

The following outlines what you can set on the **Configuration** window **Conditions** tab when working with the **Process Metallurgy Calculator**.

Configuration

Process Metallurgy Calculator 1

Conditions Options

Database: OXDEMO

Thermal control: Isothermal

Temperature: Celsius 1650.0

Pressure: Pascal 100000.0

+ -

Material: Steel Steel_BOF

Amount: Tonne 100.0 Show composition

+ -

Material: Slag Slag_BOF

Amount: Tonne 3.0 Show composition

+ -

Material: Gas Oxygen

Amount: Normal cubic meter 0.0 Show composition

Calculation Type

☐ Single ☒ One axis ☐ Grid ☐ Uncertainty

Grid Definitions

| Quantity | Min | Max | Number of steps |
|------------------------------|-----|--------|-----------------|
| Amount of Oxygen (GAS) [Nm3] | 0.0 | 7000.0 | 40 |

Help Add Predecessor Perform Tree Create New Successor

An example of the default Configuration window for a Process Metallurgy Calculator. There are many settings available depending on the parameters.



Also see ["Defining the Process Metallurgy Calculator" on page 164](#) for instructions that walk you through the steps that represent a simplified steelmaking process.

Database

The most recent available version of TCS Metal Oxide Solutions Database (TCOX) is selected by default.



The Process Metallurgy Module works with TCOX8 and newer versions of the database. The current version of the database is TCOX9.



All other users can test the module with the included OXDEMO database, which is limited to these elements: Al, C, Ca, Fe, O, S, and Si. For more information about this and other products [visit our website](#).

Thermal Control

Choose **Isothermal** or **Adiabatic**. When **Adiabatic** is selected, no global temperature is defined (as this changes during the process). Instead the initial temperature has to be defined separately for each material. Adiabatic calculations assume no heat and mass exchange with the environment during the equilibrium reaction. This is a better assumption if the process is strongly exo- or endothermic, such as typical converter processes.

Temperature

Choose a **Temperature** unit (**Kelvin**, **Celsius** or **Fahrenheit**) and then enter a numerical value in the field.

Material Groups (Steel, Slag and Gas)



For more details about these fields, see "[Defining the Process Metallurgy Calculator](#)" on page 164. See also "[Working with the Material Manager](#)" on page 176.

There are three groups to define: **Steel** (or another user-defined **Metal** group), **Slag** and **Gas**.

In the image below, the red-highlighted area is where the **Steel** material group is defined. The drop-down menu that displays *Steel_BOF* is a user-defined material. This can be defined and then saved to the material library.

When you click **Show composition** next to any material group, additional fields display (e.g. **Input type**, **Major components** and so forth) where you can further define each material group. You can add and remove materials using the Material Manager (available via the **Tools** → **Options** menu).





You can open the example project "[PMET_01: Basic Oxygen Furnace \(BOF\)](#)" on [page 288](#) from Thermo-Calc (**Help** → **Example Files** → **Process Metallurgy** → **PMET_01_Basic_Oxygen_Furnace.tcu**). Then click **Show composition** next to the **Slag** and **Gas** groups to see how the *Slag_BOF* and *Oxygen* materials are defined.

From this composition area you can click the **Save material** button to add the new material to the group's list. The newly named material composition is then available for use with that material group. In this example, the *Steel_BOF* material was defined first and then named at the end. It is now automatically available wherever you select the Steel material or need to choose quantities to plot.



The *Amount of X in Y* quantities you can choose from the various drop-down lists (such as under *Grid Definitions*) are defined as Min-Max variation of the component X in Y. If a dependent element is present that is adapted as usual.



To add one or more material groups click the green add  button. Click the red minus  button to remove a material group. The new material inherits the default settings of that group.

Configuration

Process Metallurgy Calculator 1

Conditions Options

Database: OXDEMO

Thermal control: Isothermal

Temperature: Celsius 1650.0

Pressure: Pascal 100000.0

Material: Steel Steel_BOF

Amount: Tonne 100.0 [Hide composition](#)

Input type: Mass percent Element Major component [Save material](#)

Major component:

+ - Fe 94.5

+ - C 4.5

+ - Si 1.0

Total: 100.0

Material: Slag Slag_BOF

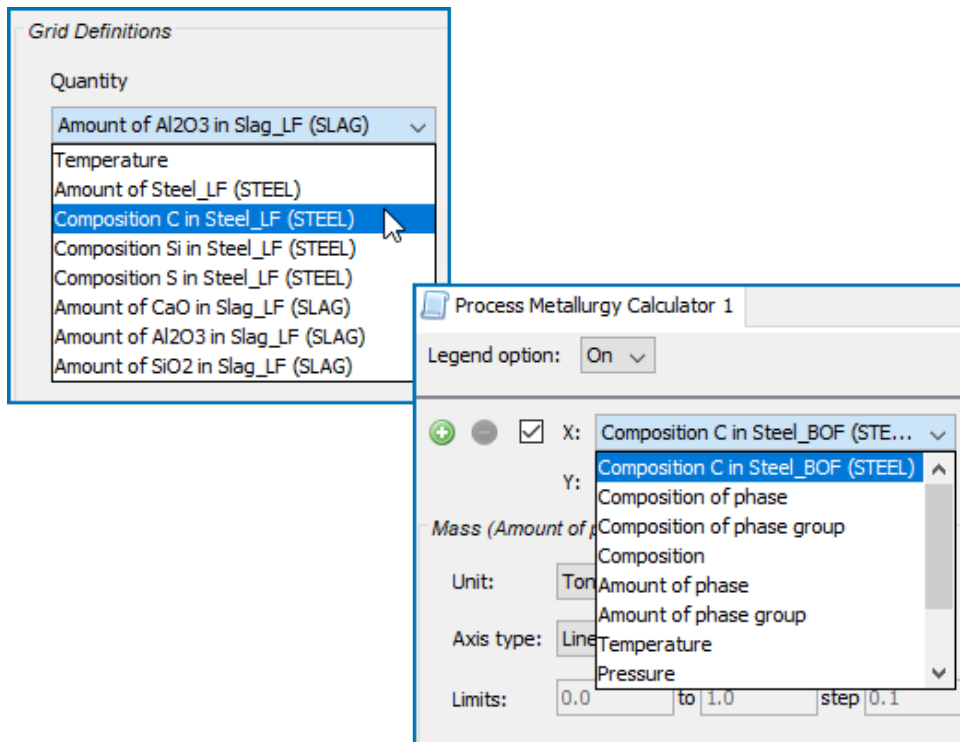
Amount: Tonne 3.0 [Show composition](#)

Material: Gas Oxygen

Amount: Normal cubic meter 0.0 [Show composition](#)

Calculation Type

The three material group areas on the Process Metallurgy Calculator where you can define components and save materials.



After defining and saving a material composition, the named material is available for selection in a variety of places such as when choosing quantities on the calculator and defining axis variables on the Plot Renderer.

Calculation Type

Single (no axes), **One axis**, **Grid** or **Uncertainty**.

► ["The Calculation Types in Graphical Mode" on page 23](#)

- Select **Single** to calculate a single point. No additional settings are required. The results from this calculation can be displayed in the **Results** window using a **Table Renderer**.
- Select **One axis** to vary a quantity on the X-axis.
- Select a **Grid** to evaluate two axis variables of the selected quantities in the specified range and number of steps.
- The **Uncertainty** calculation evaluates the equilibrium where the values of the quantities are sampled from Gaussian distributions. The **Mean** field is as defined under Condition Definitions for the respective quantity. The result is visualized as a histogram or normal probability plot by adding a Plot Render activity.

Grid Definitions (One axis or Grid)

The **Quantity** menu displays all the stepping options set up with the material groups for **Steel** (or any user-defined metal group), **Slag** and **Gas**.

For **One axis**, select a **Quantity** to vary along the X-axis, for example, **Temperature** then enter a **Min**, **Max** and **Number of steps**.

For the **Grid** calculation type, define the two axes variables using the fields and menus: **Quantity**, **Min**, **Max** and **Number of steps**. The number of steps along with the minimum and maximum values for the axes define a grid. For each grid point the selected equilibrium is evaluated.



For a **Grid**, on the Plot Renderer, you can choose to plot a *Heat map*, *Contour* or *3D* diagram.

▶ ["Heat Map, Contour and 3D Plots" on page 217](#)

Sampling of Data from Gaussian Distributions (Uncertainty)

For the **Uncertainty** calculation type, click to select the applicable check boxes under **Quantity**. The **Mean** field is for the distribution function as defined under *Condition Definitions* for the respective quantity. The default Δ Min/Max is a 95% confidence interval.

▶ ["About the Uncertainty Calculations" on page 226](#)

Sampling Parameters (Uncertainty)

For the **Uncertainty** calculation type, choose a number of **Standard deviations** where you want to **Truncate the distribution**. Choose the **Total number of samples**.

▶ ["About the Uncertainty Calculations" on page 226](#)

Options Tab

These settings are for the **Process Metallurgy Calculator** and are located on the **Configuration** window → **Options** tab.



You can change some of these settings locally for a specific Process Metallurgy Calculator or globally in the **Options** settings. To open the Options window: From the main menu select **Tools** → **Options**. Click the **Graphical Mode** tab then click **Process Metallurgy**.

▶ You can manage your saved materials from the **Tools→ Options** menu. For more information see ["Working with the Material Manager" on the next page](#).

▶ ["Conditions Tab " on page 168](#)

Process Material Equilibrium and Grid

MINIMIZATION STRATEGY

The **Minimization strategy** setting is used to ensure that the most stable minimum under the specified conditions is computed. The default uses the **Global test preferred** option.

With either the *Global* or *Local preferred* setting, the program cycles through options before it gives up:

- For **Global test preferred** the minimization starts with a global test and if that fails it runs full global minimization.
- For **Local minimization preferred** the minimization starts with a local minimization, in case of failure it tries a global test and finally a full global minimization.

If you choose **Local minimization only** or **Global minimization only**, the program just tries the one setting and gives up if it fails.



For general information about global minimization, see the topic related to the Console Mode command, ["GLOBAL_MINIMIZATION" on page 139](#).

Max no of iterations

By default, the program tries 2000 iterations before it gives up.

Max grid points (in global minimization

Coarse (2000 grid points, the default), **Medium** (20,000 grid points), **Fine** (200,000 grid points), or **Custom** (set your own number of grid points).

Required accuracy

The default is 1.0E-6. This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at

least one order of magnitude larger than the machine precision.

Smallest fraction

The default is 1.0E-16. If this value fails, the program will try other values.

This is the value assigned to constituents that are unstable.

The default value for the smallest fraction is 1E-16 for all phases except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as 1E-30.

Approximate driving force for metastable phases

The check box is selected by default, which means the metastable phases are included in all iterations. However, these may not have reached their most favourable composition and thus their driving forces may be only approximate.

Force positive definite phase Hessian

The check box is selected by default and this setting determines how to reach the minimum of an equilibrium state.

Control step size

The check box is selected by default and this setting determines how to reach the minimum of an equilibrium state.

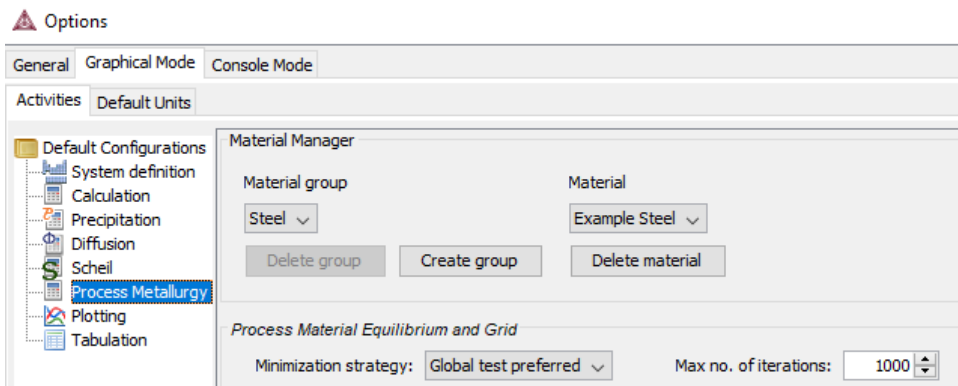
Working with the Material Manager



The Material Manager is only available for the Process Metallurgy Calculator.

Use the *Material Manager* to create and delete groups of materials and delete materials you have saved directly from the **Process Metallurgy Calculator**.

Go to the *Material Manager* from the main menu. Select **Tools → Options → Graphical Mode** and click the **Activities** tab. Then click **Process Metallurgy**. See ["Global Settings: Process Metallurgy" on page 45](#).



For frequently used materials, save the material composition for each group—Steel (or any user-defined metal), Slag or Gas—from the Process Metallurgy Calculator. Use the Material Manager to create and delete groups or delete a previously saved material.

Use the **Material group** and **Material** lists to create and delete material groups, as well as delete material compositions that are saved from the Process Metallurgy Calculator.

- **Material group:** To create or delete a group, choose it from this list, e.g. **Steel**, **Slag** or **Gas**. The *Steel* group is simply a generic **Metal** group. You can create other user-defined metal groups and then these would also be listed here. Click **Create group** or **Delete group** as required to manage the list.
- **Material:** To delete a material, choose the group type then select the material composition to delete. For example, select the **Slag** material group, then choose the **Example Slag** material and click **Delete material** to remove it from all lists.

Saving a Material

This is done directly from the **Process Metallurgy Calculator**→ **Configuration** window.

1. Add the Process Metallurgy Calculator to **My Project** directly (right-click and select it from the **Create New Activity** menu) or use the available Process Metallurgy template.
2. On the **Configuration** window, next to the **Material** group you want to define, for example Steel (or another user-defined metal group), Slag or Gas. Click **Show composition**.
3. Enter the composition and the **Major component** of the material you want to save for future use. You can alternatively select **Normalize to total of 100%** and enter the percentages for each element.
4. Click **Save material**.

-
5. In the window that opens, enter a **Material name**. Click **OK**.

When you go to the *Material Manager*, you can select this saved material from the applicable list if you need to delete it.



It is not possible to rename a saved material. You would need to recreate/redefine the material and save it again with the new name.

Deleting a Material

This is done with the *Material Manager*, located on the **Tools →Options** window.

1. After [Saving a Material](#), go to the *Material Manager*.
2. Select the **Material** group associated to the material saved previously, for example, **Steel** (or another user-defined metal group), **Slag** or **Gas**.
3. From the **Material** list, select the material you want to delete and click **Delete material**.
4. In the window that opens, click **Yes** to delete the material and **No** to cancel.

Creating a Material Group

This is done with the *Material Manager*, located on the **Tools →Options** window.

1. Go to the *Material Manager*.
2. Click **Create group**.
3. In the window that opens, select the **Material group type** (**Metal**, **Slag** or **Gas**) you want to create.
4. Enter a **Material group name**. The new group is now available to select from the **Material group** list.

Deleting a Material Group

This is done with the *Material Manager*, located on the **Tools →Options** window.

1. Go to the *Material Manager*.
2. From the **Material group** list, select the group you want to delete and click **Delete group**.
3. In the window that opens, click **Yes** or **No**.

Plot Renderer

The Plot Renderer is where you define the settings and output results in a diagram that displays in the **Results** window. The available Plot Renderer settings are based on the System Definer and/or calculator activity node predecessors such as the Equilibrium, Scheil, Binary, Ternary, and Property Model Calculators. Setting availability is also determined by the calculation type as well as if you have the add-on Diffusion, Precipitation, or Process Metallurgy Modules. If you used any of the templates, the Plot Renderer is automatically added to the Project tree.





► ["Configuration Settings" on the next page](#)

There are additional details for more advanced settings and the add-on modules:



["Plotting Options" on page 209](#), ["Diffusion Calculator Plot Renderer" on page 185](#), and ["Plot Renderer" on page 189](#)

PLOT TOOLBAR

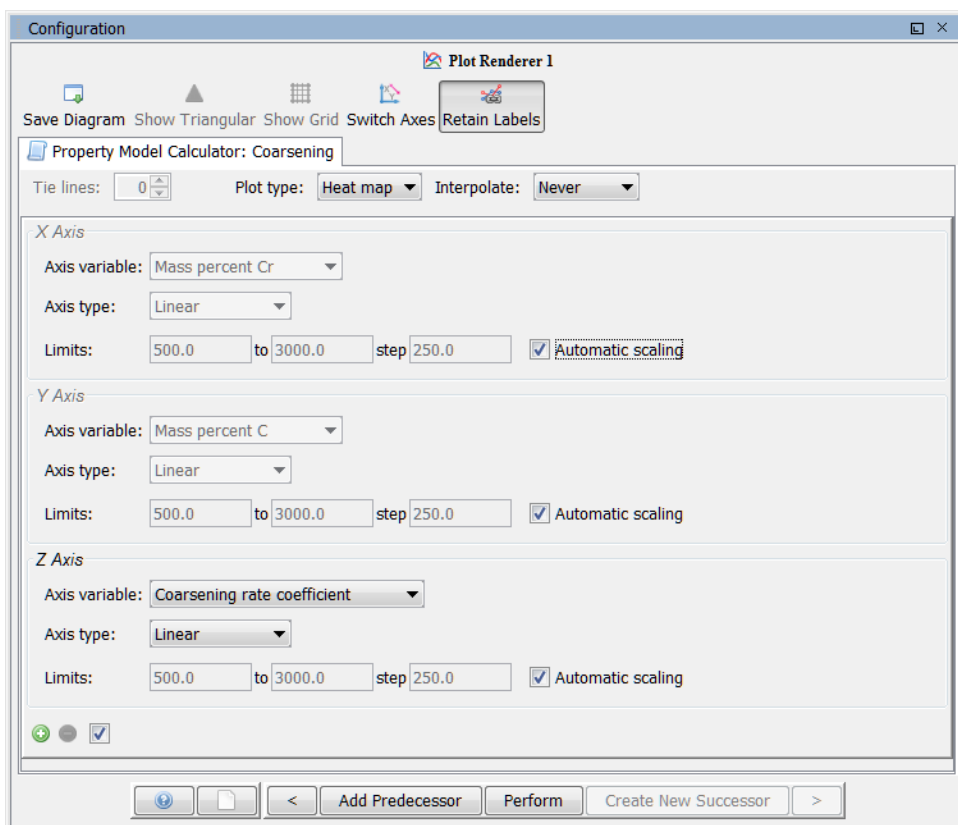
| Setting/Button | Description |
|--------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Save Diagram  | Save the plot diagram. From the Save window, choose the file type—png (the default), jpg, ps, pdf, gif, svg, or emf. For PNG and JPG files you can also change the image quality. ► "Saving and Printing the Output (Graphical Mode)" on page 205 |
| Show Triangular  | Display the diagram in triangular form, with the X-axis along the base and the Y-axis along the left side. Such a diagram is often useful if you want to plot the fractions of two components in a ternary diagram. |
| Show Grid  | Overlay a grid on the diagram. |
| Switch Axes  | Show the plotting X axis variable on the diagram's Y-axis, and the Y axis variable on the diagram's X-axis. |
| Retain Labels | Toggle the default to keep labels displaying on the plot. By default labels are retained. |

| Setting/Button | Description |
|-----------------------------------------------------------------------------------|-------------|
|  | |

Configuration Settings

- ▶ ["Working with Plots and Tables" on page 204](#)

The following is an example of the **Configuration** window for a **Plot Renderer** that is the successor to a Property Model Calculator. For some specialized calculators there is additional functionality available and described with the individual topics.



- ▶ ["Plot Settings: TTT Mode" on page 185](#), ["Diffusion Calculator Plot Renderer" on page 185](#), and ["Plot Renderer" on page 189](#)
- ▶ Also see ["Working with the Process Metallurgy Module" on page 151](#) for additional detail for the Process Metallurgy Calculator.

Examples of Calculation Type Differences

GRID

If you choose a *Grid* calculator type, select a **Plot type** and whether to **Interpolate** the data or not. With these calculation types you can choose to plot a *Heat map*, *Contour* or *3D* diagram. See ["Heat Map, Contour and 3D Plots" on page 217](#).

For a *Grid* the X- and Y-axes always represent the quantities that define the calculation axes, but you need to set a variable for the Z-axis (the axis perpendicular to the plane defined by the X- and Y-axes).

UNCERTAINTY

For an *Uncertainty* calculation type, you choose an **Axis type**: **Frequency**, **Histogram** or **Normal probability**.

There are different axis types available such as **Linear**, **Logarithmic**, **Logarithmic 10**, and **Inverse**.

Settings

The options along the top of the window are available for many of the calculation types (e.g. *Phase diagram*, *One-axis*, *Min/Max*, *Uncertainty* and so forth).

Tie-lines

Select how many tie-lines to be plotted in the diagram. Every n^{th} number of tie-line is plotted, where n is the number set here. Consequently, the higher the number, the fewer the number of plotted tie-lines in the diagram.



This setting is not available if the Plot Renderer is a successor to an Equilibrium Calculator where only one axis is defined and varied (that is, an Equilibrium Calculator that has performed a stepping calculation).

Legend option

Select whether the diagram's legend displays the **Stable phases**, the **Axis quantity**, or choose **Off** for no legend.

Legend style

You can select a Legend style for the **Stable phases** or **Axis quantity** selected for **Legend option**. Choose **None**, **All**, **Constitution description**, or **Ordering description**.

▶ ["About Legend Styles" on page 236](#)

Grouped mode or Flexible mode

For a **One axis** calculation type, the Grouped mode or Flexible mode available on the Plot Renderer help you more easily define the plot quantities.

- Use **Grouped mode** to add and configure groups of axis quantities at the same time and of the same type. For example, change units or settings in groups with similar settings like temperature units or axis types.
- Use **Flexible mode** to individually add and configure axes quantities and change the units or other associated settings one at a time.

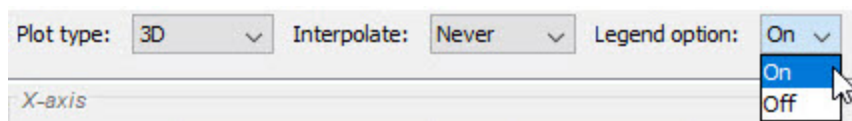
▶ ["Plot Settings: TTT Mode" on page 185](#)

Plot type (Grid)

These settings are for a **Grid** calculation type.

▶ ["Heat Map, Contour and 3D Plots" on page 217](#)

- On a **Heat map** diagram, each Z-axis variable value in the grid is represented by a colour-coded area, where dark red represents the highest Z-axis variable value and dark blue represents the lowest Z-axis variable value.
- On a **Contour** diagram, Z-axis variable values are traced with curves in the same way that height values are traced with curves on a topographical map. The colors used originate from the different data series.
- On a **3D** diagram, the 3D surface is created by Delaunay tessellation of the calculated data. The surface uses a cold to warm color map where red represents the highest Z-axis variable value and blue represents the lowest Z-axis variable value. The color map color legend can be turned on or off with the legend option.



Interpolate (Grid)

From the **Interpolate** list, choose to interpolate data **Never** (the default), **Once**, **Twice** or **3 times**. This means points are put in between calculated points in the grid and interpolated instead of calculated in the calculation engine.

Choose how many points of data to interpolate to improve curve smoothness – **Never**, **20x20**, **50x50**, or **100x100**. Try different settings for your own set of data.

Label decimal digits

Choose the number of decimal digits to display in the plot label. The default is **2**.

Label number format

Choose from **Auto** (the default), **Decimal** or **Scientific**.

Axis variable

Set the state variable you want plotted along the X-axis and the Y-axis.



If the stepping/mapping variables are changed in the Equilibrium Calculator that precedes the Plot Renderer, then the variables to be plotted along the diagram's X- and Y-axis are automatically updated to the appropriate quantities.

Axis type

Select the type of axis scale: **Linear**, **Logarithmic**, **Logarithmic 10** or **Inverse**.

Automatic scaling

The **Automatic scaling** check box is selected by default to allow the program to set the limits.

Limits

This setting is available when the **Automatic scaling** check box is cleared (the scaling is turned off).

Enter the lower and upper **Limits** of the variables to display on the axis. You can also determine the **step** size between the tick marks along each axis.



If the **Automatic scaling** is turned off (i.e. the check box is not selected) then it is important to enter a large enough number in the **step** field for the numerical values to display correctly on the axis. That is, if the step size is too small, the program ignores this setting and the axis labels will not be as expected.





For logarithmic axes, the step size is related to the exponent. For example, if the step entered is 1.0, then the exponent increases by one each time (10^{-9} , 10^{-8} , 10^{-7} and so forth).

Contour values and Use custom contour values (Z-axis, contour plots).

The **Use custom contour values** check box is available when **Contour** is selected as the **Plot type**. Select this check box to enter one or a series of numbers in the **Contour values** field. Numbers can only be separated by a space.

Add an axis and Remove this axis buttons

Use the **Add an axis**  and **Remove this axis**  buttons to add additional X- and/or Y-axes to a plot or to merge plots (to overlay one plot with another in the same diagram). When merging plots, you define this variable as the Z-axis.

▶ ["Plotting Options" on page 209](#)

Slag Property Options (Process Metallurgy)

For the **Process Metallurgy Calculator** when you are selecting axis variables on the Plot Renderer, there is the option to choose **Slag property**. The associated quantity that you select from the next drop-down list has these options to choose: **All**, **B2**, **B3**, **B4**, **Bas2**, **Bells ratio**, **Ls**, or **Log10 (Sulphur capacity)**.

Also choose **In liquid slag only**, **In solid slag only** or **In all slag**.

▶ References and equations for these properties are described in ["Process Metallurgy Slag Properties" on page 160](#).

Unit (Process Metallurgy)

For the **Process Metallurgy Calculator** select a **Unit** for the quantity to plot: **Tonne**,

Kilogram, Gram or Pound

Plot Settings: TTT Mode

- ▶ ["Configuration Window Settings" on page 106](#) and ["Configuration Settings" on page 180](#)
- ▶ ["About the Steel Property Models in Thermo-Calc" on page 99](#)

Use TTT mode to define the **Temperature** on the y-axis and **Time** on the x-axis for all selected quantities. The **TTT mode** is available for a **Plot Renderer** when it is a successor to a Property Model Calculator that meets the following requirements:

- If you are using both the **Martensite temperatures** and **Pearlite** property models together this mode is available. These models also require specific maintenance and database licenses.
- A **One axis Calculation Type** is selected.

An example of when to use TTT mode is to configure the **Temperature Unit** and **Axis type** at the same time for both the *Ms* and *Growth rate* quantities. This mode is available when both time and temperature quantities are selected and set up to plot a Time-Temperature-Transformation (TTT) diagram.

When you add the **Steel Library - TTT Template** this mode is set by default on the Plot Renderer (renamed TTT in the template). It is also available if a user-defined property model has both Time and Temperature quantities defined, for example if you create your own property model with the Property Model Development Framework. That is, if you select or create any model where the resulting combination of stepping-quantity and result-quantities has both time and temperature definitions.

- ▶ ["Steel Library TTT Diagram Template" on page 33](#)

Diffusion Calculator Plot Renderer

- ▶ ["Conditions Tab Settings" on page 112](#) and ["Configuration Settings" on page 180](#)

The following is information about the settings available in both Simplified and Advanced mode for a Plot Renderer when it is a successor to a **Diffusion Calculator**.

Simplified Mode

When you open the Diffusion Calculator Plot Renderer, it defaults to **Simplified mode**. Use this mode to define the most common axis variables. The software automatically sets the correct **Plot condition** and **Independent variable**. Use the **Advanced mode** to have more

flexibility.



When you click the **Switch to advanced mode** button, this expands the variable options available from both the X-axis and Y-axis lists. Otherwise the axis variables default to the most logical combination.

X-AXIS VARIABLE

Select the variable for the x-axis: **Distance** or **Time**.

- For **Distance** also choose a unit (**m**, **μm**, or **nm**) and what region to include. The list contains the regions defined on the Diffusion Calculator or you can choose **All regions**.
- For **Time** choose a unit (**Seconds**, **Minutes**, **Hours**, or **Days**).

Y-AXIS VARIABLE

Select the variable to plot on the y-axis. The available options are based on choices such as whether **Distance** or **Time** is chosen for the x-axis, whether isothermal or non-isothermal is selected, whether there is a homogenization solver, or if there is one or more regions.

Distance along the x-axis

If **Distance** is plotted along the x-axis, then by default the **Composition** is plotted along the y-axis.

- From the center list, choose the component to plot, or select **All**.
- From the next list, choose the unit to be **Mass percent**, **Mole percent**, **Mass fraction**, **Mole fraction**, or **u-fraction**.

Time along the x-axis (one region)

If **Time** is plotted along the x-axis, then choose the y-axis variable to plot plus the additional settings:

- **Total phase fraction: By volume** or **By mass**. Then select a phase from the list.
- **Total fraction of element: By mole** or **By mass**. Then select a component from the

list.

- **Total fraction of element in phase: By mole or By mass.** Then select a component and a phase from the lists.
- For a non-isothermal thermal profile **Temperature** is available: **Kelvin, Celsius, or Fahrenheit.**

Distance along the x-axis (Homogenization)

If **Distance** is plotted along the x-axis and a Homogenization solver is being used, then choose **Composition** or **Phase fraction** to plot on the y-axis. Then select the applicable settings.

- Choose the component to plot, or select **All** and the unit **Mass percent, Mole percent, Mass fraction, Mole fraction, or u-fraction.**
- Choose **By mole** or **By mass** then select a component from the list.

Time along the x-axis (two or more regions)

If **Time** is plotted along the x-axis, then choose the y-axis variable to plot plus the additional settings:

- **Total phase fraction: By volume or By mass.** Then select a phase from the list.
- **Total fraction of element: By mole or By mass.** Then select a component from the list.
- **Total fraction of element in phase: By mole or By mass.** Then select a component and a phase from the lists.
- **Composition at interface: Mass percent, Mole percent, Mass fraction, Mole fraction.** Then choose a **Region** and whether it is **Upper** or **Lower** and a component.
- **Position of interface:** Choose a unit (**m, μm , or nm**) and the interface.
- **Velocity of interface:** Choose a unit (**m, μm , or nm**) and the interface.
- **Width of region:** Choose a unit (**m, μm , or nm**) and the interface.
- For a **Non-isothermal** profile, **Temperature** is available. Choose a unit **Kelvin, Celsius or Fahrenheit.**

AXIS TYPE

Select the type of axis scale: **Linear, Logarithmic, Logarithmic 10 or Inverse.**

LIMITS

Specify the range along the axis to show in the plot. In the fields, enter the minimum and maximum values of the axis variable. You can also determine the **step** size between the tick marks along each axis.

Select the **Automatic scaling** check box to allow the program to set the limits.



TIME



An alternative **Time** setting is available in Advanced mode.

When the x-axis variable is **Distance**, choose a **Time** unit (**Seconds**, **Minutes**, **Hours**, or **Days**). Enter a numerical value.

ADD AND REMOVE AXES

Use the **Add an axis**  and **Remove this axis**  buttons to add additional X- and/or Y-axes to a plot or to merge plots (to overlay one plot with another in the same diagram).

Advanced Mode

Choose **Advanced mode** to access settings that enable you to manually select any combination of axis variables, **Plot condition** and **Independent variable**. Examples of advanced plot options are activity of a component at an interface, diffusivities, and diffusion paths. Also user-defined functions can be used as plot variable where Console Mode syntax is used to define functions. In some cases, sensible default values are selected, but they can be changed according to your needs.

PLOT AXIS SETTINGS IN ADVANCED MODE

- If any plot axis variable of the type **Integral** is selected, then the plot condition is set to **Integral** and the Independent variable is set to **Time**.
- If a plot axis variable is set to **Time** then the plot condition is set to **Time** and the Independent variable is also set to **Time**.
- If a plot axis variable is set to **Distance** then the plot condition is set to **Distance** or **Interface** and the Independent variable is set to **Distance**.

| Plot condition | Independent Variable settings based on the Plot condition |
|--------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Time: Choose a unit (Seconds, Minutes, Hours, or Days). Enter a numerical value. | The default is Distance : Choose a Global or Local distance. A Global distance is counted from the rightmost interface of the system. A Local distance is counted from the lower interface of the Region selected. You can also choose Time , which requires no further settings. |
| Distance: Choose a specific Region from the list or use the default All regions . | The default is Time and there are no further settings. You can also choose a Global or LocalDistance . A Global distance is counted from the rightmost interface of the system. A Local distance is counted from the lower interface of the Region selected. |
| Interface: From the lists choose a Region and whether it is the Upper or Lower region. | The default is Distance : Choose a Global or Local distance. A Global distance is counted from the rightmost interface of the system. A Local distance is counted from the lower interface of the Region selected. You can also choose Time , which requires no further settings. |
| Integral | The default is Time and there are no further settings. You can also choose a Global or LocalDistance . A Global distance is counted from the rightmost interface of the system. A Local distance is counted from the lower interface of the Region selected. |

Plot Renderer

► ["Conditions Tab Settings" on page 132](#) and ["Configuration Settings" on page 180](#)

The following is information about the settings available for a Plot Renderer when it is a successor to a **Precipitation Calculator**.

There are also specific settings related to non-isothermal simulations that are detailed in this topic.

Plot Settings

Legend option

Select whether the diagram's legend displays **On** or **Off**.

Axis variable

Set the state variable you want plotted along the X-axis and the Y-axis.

Select the **Separate multimodal PSD** check box to enter settings for **Points**, **Excess kurtosis**, **Valley depth ratio** and **Minimum peak**.

▶ See "[Non-Isothermal Simulations](#)" on the next page for definitions.

Axis type

Select the type of axis scale: **Linear**, **Logarithmic**, **Logarithmic 10** or **Inverse**.

Limits



Specify the range along the axis to show in the plot. In the fields, enter the minimum and maximum values of the axis variable. You can also determine the **step** size between the tick marks along each axis.

Select the **Automatic scaling** check box to allow the program to set the limits.

Unit (*Time X Axis*)

Choose a **Unit** : **Seconds**, **Hours**, or **Days**.

Add an axis and Remove this axis buttons

Use the Add an axis  and Remove this axis  buttons to add additional X- and/or Y-axes to a plot or to merge plots (to overlay one plot with another in the same diagram). When merging plots, you define this variable as the Z-axis.

Axis Variables

- **Mean radius:** Spherical radius of average volume of all particles for a specific phase and nucleation type, regardless of their actual shapes.
- **Critical radius:** Spherical radius of critical nuclei for a specific phase and nucleation type.
- **Matrix composition:** Instantaneous compositions of the matrix phase.
- **Precipitate composition:** To track the instantaneous composition of precipitate particles. In particular, it is useful to distinguish different composition sets of the same phase (for example, FCC_A1#2 and FCC_A1#3). Further choose **Solutes** or **All**.
- **Number density:** Instantaneous number of particles per unit volume for a specific phase and nucleation type.

- **Size distribution:** Number of particles varying with their sizes per unit volume per unit length, for a specific phase and nucleation type, at a specific time.
- **Number density distribution:** Retrieve the number density (number of particles per unit volume) of precipitates distributed in different particle sizes.
- **Volume fraction:** Instantaneous volume fraction for a specific phase and nucleation type.
- **Nucleation rate:** Instantaneous number of nuclei per unit volume per unit time for a specific phase and nucleation type.
- **Normalized driving force:** Instantaneous nucleation driving force per unit mole of elements for a specific phase and nucleation type. It is normalized with RT and therefore, dimensionless.
- **Mean cubic factor:** Average cubic factor of cuboid particles. Available only when cuboid is selected as the **Morphology**.

The following settings area available as indicated when **Needle**, **Plate** or **Cuboid** are selected as the **Morphology** in the *Precipitate Phase* section on the Precipitation Calculator.

- **Cubic factor distribution:** Variation of cubic factor with particle size at a specific time. Available with a cuboid morphology.
- **Mean aspect ratio:** Average aspect ratio of non-spherical particles. Available with a needle or plate morphology. Note that this is always larger than 1, where 1 = a sphere.
- **Mean particle length:** Diameter of non-spherical particles along the longer axis. Available with a needle or plate morphology.
- **Aspect ratio distribution:** Variation of aspect ratio with particle size at a specific time. Available with a needle or plate morphology.

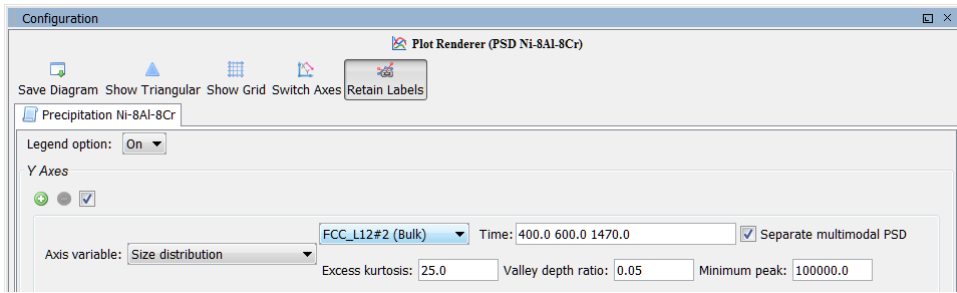
Non-Isothermal Simulations

When doing non-isothermal simulations it is common that particles grow in different generations. This results in multi-modal size distributions. To correctly estimate the properties of these different generations of particles you need to separate the peaks of multi-modal distributions.

Separate multimodal PSD

When the **Separate multimodal PSD** check box is selected on a Plot Renderer activity for the Precipitation Calculator, the size distribution is evaluated at the given time steps and checked for multi-modal peaks. These are separated and used to calculate the specified

property.



It can be applied on the following plot properties:

- Mean radius
- Size distribution
- Number density
- Volume fraction

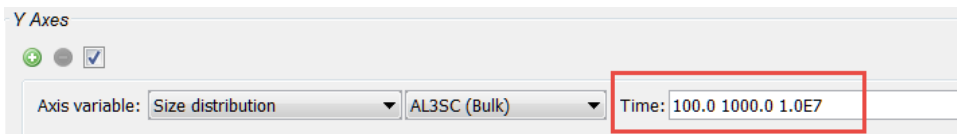
Points

This field is available when **Mean radius**, **Number density** or **Volume fraction** is selected as the **Axis variable**. Since the evaluation of multi-modality at each time step is costly, you can specify how many evaluation **Points** to use. The points are geometrically distributed over the time scale where nucleated particles are found. The default is 40 points.

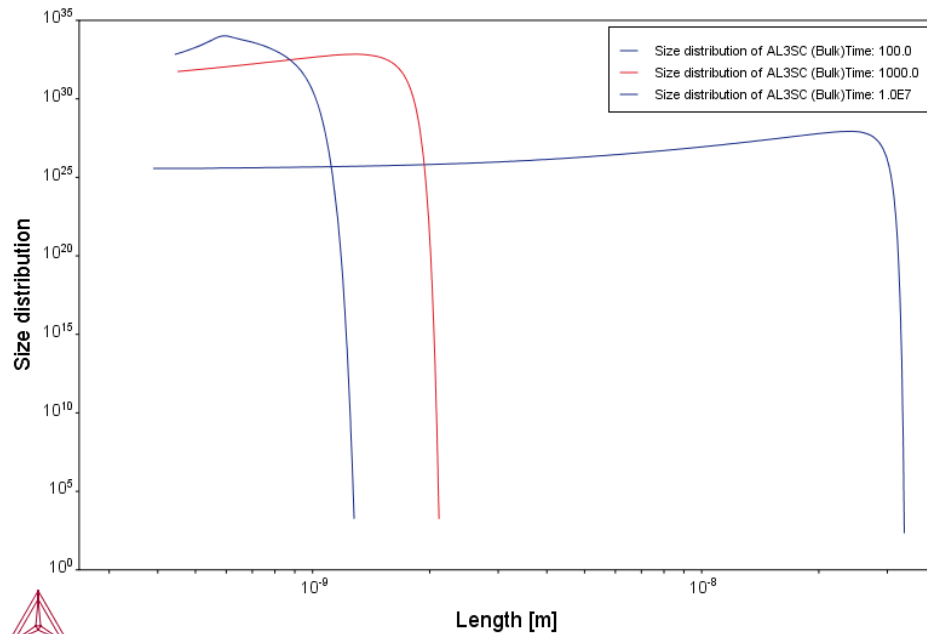
Time

This field is available when **Size distribution** or **Number density distribution** is selected as the **Axis variable**. Enter one or a series of numbers in the field, separated by a space.

For example, if you enter 100.0, 1000.0 and 1.0E7 in the field:



When you click **Perform** the times are plotted:



Excess Kurtosis

The **Excess kurtosis** number specifies the sensitivity when the program evaluates whether a curve is bimodal or not. The evaluation process calculates the excess kurtosis of the given size distribution and compares it with the input value. If the value is lower than the given value, the distribution is split. The excess kurtosis is a statistical measure that measures how *peaked* and *how heavy tail* a distribution has. For the definition used see <http://en.wikipedia.org/wiki/Kurtosis>. The default is 25.0.

Minimum Separation Limit (Valley Depth Ratio)

The **Minimum Separation Limit** is a rough method to prevent that noise or wiggles are interpreted as different distributions. If a local minima is encountered above this value the following peak is not interpreted as a new distribution. The valley depth ratio is the ratio of the minimum separation limit to the peak value. The default is 0.01.

Minimum Peak

Any separated peak below the entered **Minimum peak** value is removed. The default is 100000.0.

Table Renderer

A **Table Renderer** visualizes calculation results in a table. Several Table Renderer activities (as well as Plot Renderer activities) can be shown in the Results window as different tabs.

You can add the Table Renderer directly (right-click a calculator node and select it from the **Create New Successor** menu) or use a variety of the available templates to automatically add the node. For example, the **Single Point Equilibrium** and **Quick Start** templates.

- ▶ For details about the templates, see ["The Quick Start Wizard and Templates" on page 26](#) and ["Creating a Project from a Template" on page 30](#).

You can only successfully tabulate the results of a single equilibrium calculation or a stepping operation. The tabulated data from an equilibrium calculation is different from the tabulated data from a stepping calculation. Examples are given below.

- ▶ The settings are described in the section ["Configuration Settings" on page 197](#).

RESULTS FROM AN EQUILIBRIUM CALCULATION

The following tab shows the result of an equilibrium calculation (from example ["T_01: Calculating a Single-Point Equilibrium" on page 240](#)).

| Table Renderer 1 | | | | |
|--------------------|----------------------|----------------------|-----------------|------------------|
| System | | | | |
| Moles | 1.00000 | | | |
| Mass | 55.64392 | [g] | | |
| Temperature | 1000.00000 | [K] | | |
| Total Gibbs Energy | -42140.55264 | [J] | | |
| Enthalpy | 24707.16903 | [J] | | |
| Volume | 7.29746E-6 | [m3] | | |
| <i>Component</i> | <i>Mole Fraction</i> | <i>Mass Fraction</i> | <i>Activity</i> | <i>Potential</i> |
| Fe | 0.99537 | 0.99900 | 0.00619 | -42277.77189 |
| C | 0.00463 | 0.00100 | 0.21818 | -12658.35450 |

Stable Phases

| | <i>Moles</i> | <i>Mass</i> | <i>Volume Fraction</i> | |
|----------------------|----------------------|----------------------|------------------------|--------------------------------|
| BCC_A2#1 | 0.99609 | 55.59691 | 0.99711 | Composition and constitution ▼ |
| Composition | | | | |
| <i>Component</i> | <i>Mole Fraction</i> | <i>Mass Fraction</i> | | |
| Fe | 0.99928 | 0.99984 | | |
| C | 0.00072 | 0.00016 | | |
| Constitution | | | | |
| | $(Fe)_1 (C, VA)_3$ | | | |
| | <i>Constituent</i> | <i>Site Fraction</i> | | |
| <i>Sublattice 1:</i> | | | | |
| | Fe | 1.00000 | | |
| <i>Sublattice 2:</i> | | | | |
| | VA | 0.99976 | | |
| | C | 0.00024 | | |

For each stable phase listed, from the **Composition and constitution** menu you can select the information to view. In this example, the maximum amount of information is shown and includes details about both composition and constitution for **BCC_A2#1**.



The default for the Phase description detail can be changed globally. To open the Options window: From the main menu select **Tools → Options** and click the **Activities** tab. Then click **Tabulation**.

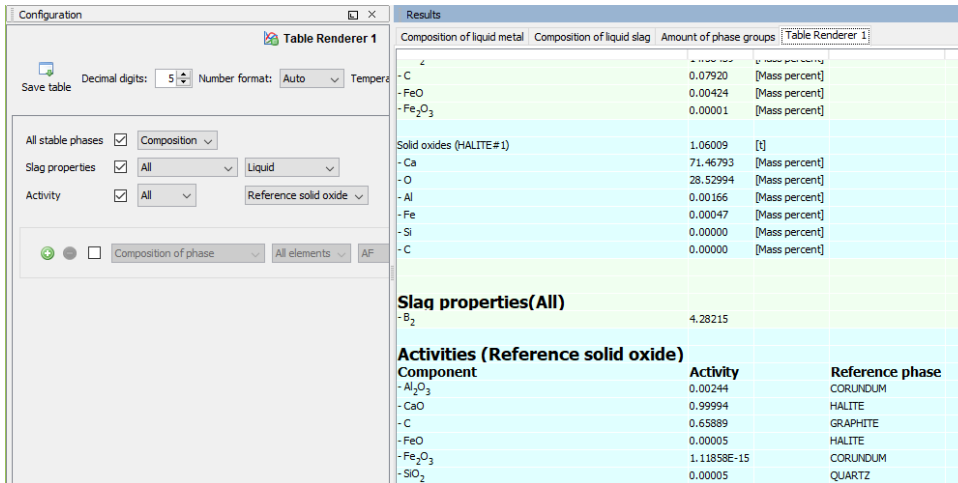
RESULTS FROM A STEPPING OPERATION

The **Table Render 1** tab in the example shows the results of a stepping calculation (from example "[T_02: Stepping in Temperature in the Fe-C System](#)" on page 242).

| Results | | | | |
|---------------------------------------------------------------------|------------------------|------------------------|------------------------|--------------------------|
| <div> <div>Plot Renderer 1</div> <div>Table Renderer 1</div> </div> | | | | |
| Temperature [K] | Amount of BCC_A2 [mol] | Amount of LIQUID [mol] | Amount of FCC_A1 [mol] | Amount of GRAPHITE [mol] |
| 1000.00000 | 0.99609 | | | 0.00391 |
| 1010.00000 | 0.99618 | | | 0.00382 |
| 1011.17278 | 0.99620 | | | 0.00380 |
| 1011.17278 | 0.99620 | | 0.00000E0 | 0.00380 |
| 1011.17278 | 0.87364 | | 0.12636 | 0.00000E0 |
| 1011.17278 | 0.87364 | | 0.12636 | |
| 1020.00000 | 0.86046 | | 0.13954 | |
| 1030.00000 | 0.84331 | | 0.15669 | |
| 1040.00000 | 0.82356 | | 0.17644 | |
| 1050.00000 | 0.80082 | | 0.19918 | |
| 1060.00000 | 0.77395 | | 0.22605 | |
| 1070.00000 | 0.74180 | | 0.25820 | |

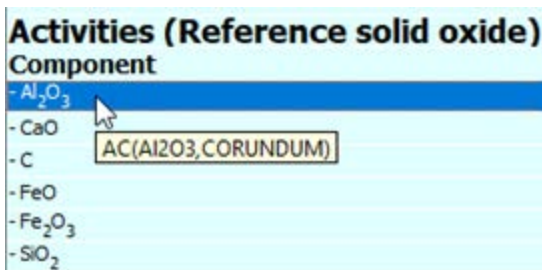
PROCESS METALLURGY MODULE SINGLE EQUILIBRIUM

When you use a **Process Metallurgy Calculator**, there is a variety of additional information you can display in the table such as the **Slag properties** (see "[Process Metallurgy Slag Properties](#)" on page 160 for equations and references) and the **Activities**.



| Composition of liquid metal | | | Composition of liquid slag | | | Amount of phase groups | | |
|-------------------------------------------|-------------|-----------------|----------------------------|-----|--|------------------------|--|--|
| C | 0.07920 | [Mass percent] | | | | | | |
| FeO | 0.00424 | [Mass percent] | | | | | | |
| Fe ₂ O ₃ | 0.00001 | [Mass percent] | | | | | | |
| Solid oxides (*HALITE#1) | | | 1.06009 | [t] | | | | |
| Ca | 71.46793 | [Mass percent] | | | | | | |
| O | 28.52994 | [Mass percent] | | | | | | |
| Al | 0.00166 | [Mass percent] | | | | | | |
| Fe | 0.00047 | [Mass percent] | | | | | | |
| Si | 0.00000 | [Mass percent] | | | | | | |
| C | 0.00000 | [Mass percent] | | | | | | |
| Slag properties(All) | | | 4.28215 | | | | | |
| Activities (Reference solid oxide) | | | | | | | | |
| Component | Activity | Reference phase | | | | | | |
| Al ₂ O ₃ | 0.00244 | CORUNDUM | | | | | | |
| CaO | 0.99994 | HALITE | | | | | | |
| C | 0.65889 | GRAPHITE | | | | | | |
| FeO | 0.00005 | HALITE | | | | | | |
| Fe ₂ O ₃ | 1.11858E-15 | CORUNDUM | | | | | | |
| SiO ₂ | 0.00005 | QUARTZ | | | | | | |

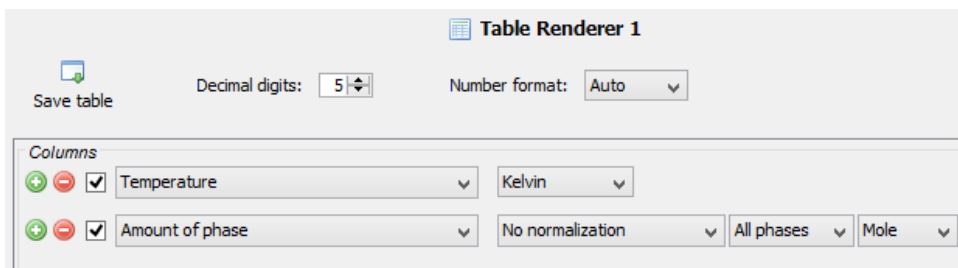
For the activities in the table, you can hover over the Component and the syntax of the activity displays.



| Component |
|--------------------------------|
| Al ₂ O ₃ |
| CaO |
| C |
| FeO |
| Fe ₂ O ₃ |
| SiO ₂ |

Configuration Settings

The **Table Renderer** settings are done on the **Configuration** window. Depending on what calculator node the table is a successor to, you can have different settings available. For most tables, this is where you set the level of detail for the columns as shown in the figure.



| Table Renderer 1 | | | |
|-------------------------------------|-------------------|---------------------|-----------------|
| Save table | Decimal digits: 5 | Number format: Auto | |
| Columns | | | |
| <input checked="" type="checkbox"/> | Temperature | Kelvin | |
| <input checked="" type="checkbox"/> | Amount of phase | No normalization | All phases Mole |

Save the Table

To save all the data in a table as a plain text file (.txt), Hyper Text Markup (.html), or Excel (.xls) format, in the **Configuration** window click **Save table** or in the **Results** window right-click in the table and select **Save As**.

To copy the data from a single cell of a table to the clipboard, right-click the cell and select **Copy**. To copy the whole table to the clipboard, select **Copy all**.



The data saved is what is shown in the **Table Renderer** tab on the **Results** window. If data is calculated but not displayed it is not saved.

Number of Decimal Digits and Number Format

The table results can be presented in ordinary decimal number format or with normalized scientific notation. Choose **Scientific** or **Decimal** to increase or decrease the number of **Decimal digits** used in the table. The default is 5 digits. The **Number format** defaults to **Auto** to use the most appropriate format based on the tabulated data.



The defaults for these settings can be changed globally. From the main menu select **Tools** → **Options** and click the **Activities** tab. Then click **Tabulation**.

Process Metallurgy Settings

For the **Process Metallurgy Calculator** there are additional settings available.

Configuration

Table Renderer 1

Save table

Decimal digits: 5

Number format: Auto

Temperature unit: Kelvin

Mass unit: Tonne

All stable phases ☒ Composition

Slag properties ☒ All In liquid slag only

Activity ☒ All Reference solid oxide

☒ ☐ ☐ Composition of phase All elements AF Mass percent

Choose a **Temperature unit**: Kelvin, Celsius or Fahrenheit.

Choose a **Mass unit** : **Tonne**, **Kilogram**, **Gram** or **Pound**.

Select the **All stable phases** check box and choose **Composition** or **Condensed** from the list.

Select the **Slag properties** check box and choose the associated quantity from the next drop-down list: **All**, **B2**, **B3**, **B4**, **Bas2**, **Bells ratio**, **Ls** , or **Log10 (Sulphur capacity)**.

Also choose **In liquid slag only**, **In solid slag only** or **In all slag**.

▶ Details, including references and equations, are described in ["Process Metallurgy Slag Properties" on page 160](#).

Select the **Activity** check box then from the first list choose a component (or keep the default **All**). Then from the second drop-down list select **Reference solid oxide** or **Reference liquid slag**.


The activity is always given relative to a phase. The liquid slag is always the IONIQ_LIQ phase. The composition set of ION_LIQ depends on the calculation and the slag always contains a high amount of oxygen. The reference phase for the solid oxides depends on the components and it is always listed in the table.



Experimental File Reader

The Experimental File Reader activity can only be created from the top My Project node. This activity allows you to read an experimental data file (*.EXP). This type of file has information specifying a plotted diagram, written in the DATAPLOT graphical language. From this activity node you can plot the EXP file or save a copy of the file to another location.

► ["Creating Activities and Successors" on page 13](#) and ["Plotting Experimental Data Files" on page 4](#) in the *DATPLOT User Guide* included with this documentation set.

PLOTTING AN EXPERIMENTAL DATA FILE

1. Right-click **My Project** and from the **Create New Activity** submenu choose **Experimental File Reader**.
2. In the **Configuration** window in the **EXP file** field, enter the name of the EXP file to plot. Or click the **Select Exp file**  button to navigate to a location on the computer.
3. Right-click the **Experimental File Reader** node and from the **Create New Successor** submenu choose **Plot Renderer**.

If the source EXP file is changed, you can also click the **Reload the selected EXP file from disk**  button to refresh the data. If you want to save or export the loaded file, click the **Save EXP file**  button, then navigate to where you want to save it and give it a file name.

4. In the **Configuration** window click **Perform** or right-click the **Plot Renderer** node and select **Perform**.

Scheduler and Event Log Windows

In this section:

| | |
|---------------------------|-----|
| Using the Scheduler | 202 |
| Event Log Window | 203 |

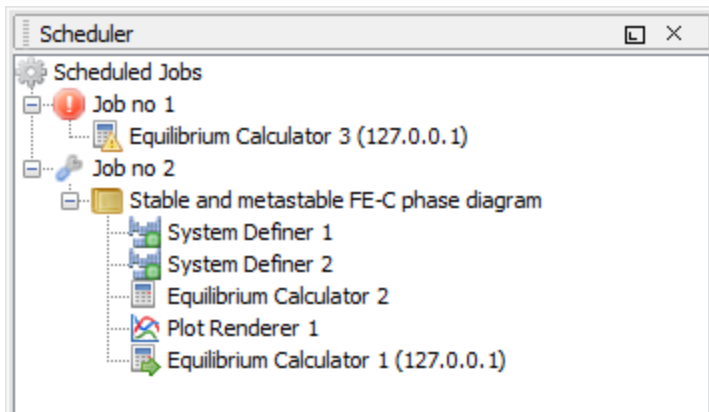
Using the Scheduler

The **Scheduler** window has activity information about current or scheduled jobs. A *job* is any activity you have selected to be performed. The Scheduler also indicates if there is an error during a job and when a job has stopped. If you have set an activity, tree or project to be performed at a later time then this is also listed.

ABOUT THE SCHEDULER JOBS

- Whenever you trigger the performance of a whole project, tree or individual activity, all the activities to be performed are shown under a job heading.
- When all the activities belonging to a job are completed the job and its activities disappear from the Scheduler window.
- If there is an error during the performance of an activity, icons for that job and activity remain in the Scheduler window until removed.

► ["Node or Window Status Markers" on page 17](#)



MANAGING THE SCHEDULE

In the Scheduler window, you can cancel scheduled jobs, remove errors and show information about errors.

- To cancel all jobs: Right-click the **Scheduled Jobs** label or the cogwheel icon, and select **Cancel All Jobs**
- To remove (clear) all failed activities and jobs: Right-click the **Scheduled Jobs** label or the cogwheel icon, and select **Clear All Errors**
- To cancel a specific job: Right-click the job label (for example, **Job no 1**) and select

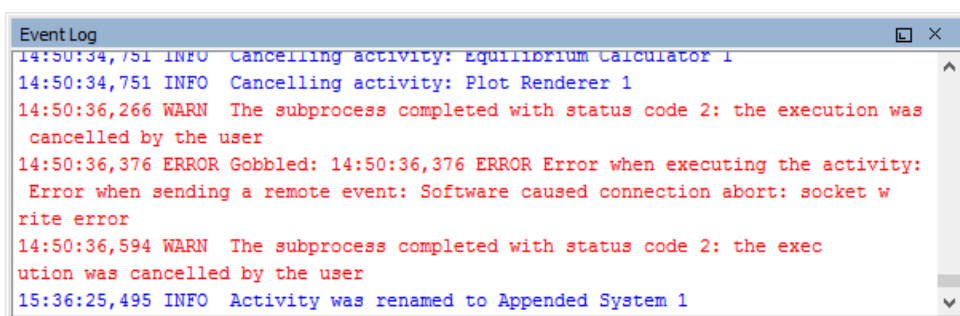
Cancel Job

- To remove (clear) a specific failed job: Right-click the job label (for example, **Job no 1**) and select **Cancel Job**
- To open a window with error details: Right-click the label for the failed job (for example, **Job no 1**), and select **Show Error Log**

Event Log Window

The **Event Log** window is closed by default. Information about what Thermo-Calc is processing or doing is in blue text and error or warning messages are in red text.

▶ ["Changing Global Settings" on page 36](#)



- To open the Event Log window: Click the **Event Log** window once to expand it or select it from the **Window → Event Log** menu. Double-clicking the window maximizes it
- To specify the level of detail in the Event Log: From the main menu select **Tools → Options**. In the **General** tab set the **Log level** slide bar to anything between **Debug** (most detailed) and **Error** (least detailed)

Working with Plots and Tables

In this section:

| | |
|-------------------------------------------------------|-----|
| Performing Projects, Trees and Activities | 205 |
| Saving and Printing the Output (Graphical Mode) | 205 |
| Zooming In and Out | 207 |
| Plotting Options | 209 |
| Plot and Table Formatting | 232 |

Performing Projects, Trees and Activities

You can trigger the performance of an activity (also called a *job*) and all the activities below it in the same tree in either the **Project** or **Configuration** window. In the Project window you can also perform a single activity without performing its successors or perform the whole project (all the activity trees).

In the **Configuration** window, click **Perform Tree** to perform the currently selected activity and all the activities below it. If there are no activities below the selected activity, then the button says **Perform** instead.



All activities that must be completed as prerequisites are automatically performed first. For example, if you Perform Tree for a Plot Renderer, then the predecessors, Equilibrium Calculator and System Definer, are automatically performed before the Plot Renderer.

In the Project window, you can do any of the following:

- Perform an activity: Right-click the activity and select **Perform Now**, or **Perform Later** and schedule a time to perform the activity
- Perform an activity and all activities below it in the tree: Right-click any node in the tree and select **Perform Tree Now**. Or select **Perform Tree Later** and schedule a time for all activities in the tree to be performed
- Perform a project: Right-click **My Project** and select **Perform Now** or **Perform Later** and schedule a time to perform all project activities in the tree



If there is an error during the performance of an activity, icons display status markers, which are described in ["Node or Window Status Markers" on page 17](#).

Saving and Printing the Output (Graphical Mode)



["Global Settings: Graphical and Console Mode Plotting" on page 47](#)



Output can refer to results in the form of tabulated data in a table or a diagram.



The terms *diagram* and *plot* are interchangeable. The commands in Console Mode generally use the term diagram and in Graphical Mode it is also called a plot (e.g. the Plot Renderer).

In Graphical Mode the output is displayed in the **Results** window. The output can be in the form of a table when you use the ["Table Renderer" on page 194](#) or a diagram (plot) when you use a ["Plot Renderer" on page 179](#). In both cases you can save from the **Configuration** or **Results** windows. You can print the table or diagram from the **Results** window.

Saving Diagrams

You can save the output in a variety of file formats. For JPG and PNG images you can also adjust the image quality.



In Console Mode, the diagram is output to the **Console Results** window after using the PLOT_DIAGRAM command.



In Graphical Mode, the diagram is output to the **Results** window after performing a tree that includes a Plot Renderer.

1. In the **Results** window, right-click the diagram and select **Save as**.

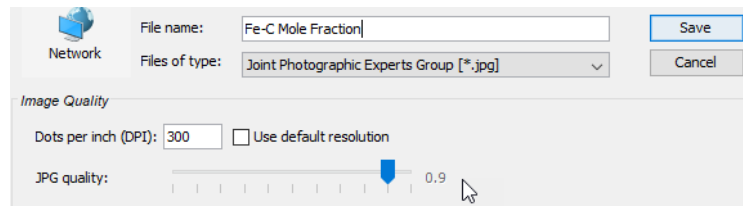


In the Graphical Mode **Configuration** window you can also click the **Save Diagram** (or **Save table**) buttons to open the **Save** window.

2. In the **Save** window:

- a. Navigate to where you want to save the diagram.
- b. Enter a **File name**.
- c. From the **Files of type** list choose **png**(the default), **jpg**, **ps**, **pdf**, **gif**, **svg**, or **emf**.
- d. For PNG and JPG files only, under the **Image Quality** section, choose to improve the resolution of the image. For JPG files you can also adjust the file size.
 - To change the resolution of a PNG or JPG image, click to clear the **Use screen resolution** check box. Then enter a numerical value in the **Dots per inch (DPI)** field.
 - For JPEG files, you can also use the slider to choose a number between 0 and 1 for the **JPG quality**. The default is 0.9. The lower the number,

the smaller the file.



e. When you are ready, click **Save**.

Saving Tables

You can save the table output in different file formats.



In Graphical Mode, the diagram is output to the **Results** window after performing a tree that includes a Table Renderer.

1. In the **Results** window, right-click the table and select **Save as**. Or in the Graphical Mode **Configuration** window click the **Save table** button.
2. In the **Save** window:
 - a. Navigate to where you want to save the table.
 - b. Enter a **File name**.
 - c. From the **Files of type** list choose **txt**(the default), **html**, or **xls**.
 - d. When you are ready, click **Save**

Printing Output

In the **Results** window, right-click the table or diagram and choose **Print**. Select additional settings as required on the **Print** window.

Zooming In and Out

In the **Results** window (where the plots are):

- Use the mouse scroll wheel to zoom in and out.
- Click and drag the mouse from left to right to highlight an area of the plot to zoom into a specific point. Use the scroll wheel to continue zooming in or out.

Resetting a Plot to the Default View

- For 2D plots, click and drag the mouse from right to left.
- For 2D and 3D plots, click **Perform Tree** to regenerate the plot in the **Results** window.

▶ ["Rotating 3D Plots" on page 231](#)

In the **Project** window (where the activity nodes are):

- Right-click and select **Zoom In** or **Zoom Out**.
- To go back to the default zoom, select **Reset Zoom**.

Plotting Options

The ["Plot Renderer" on page 179](#) is a dynamic activity node with options such as being able to:

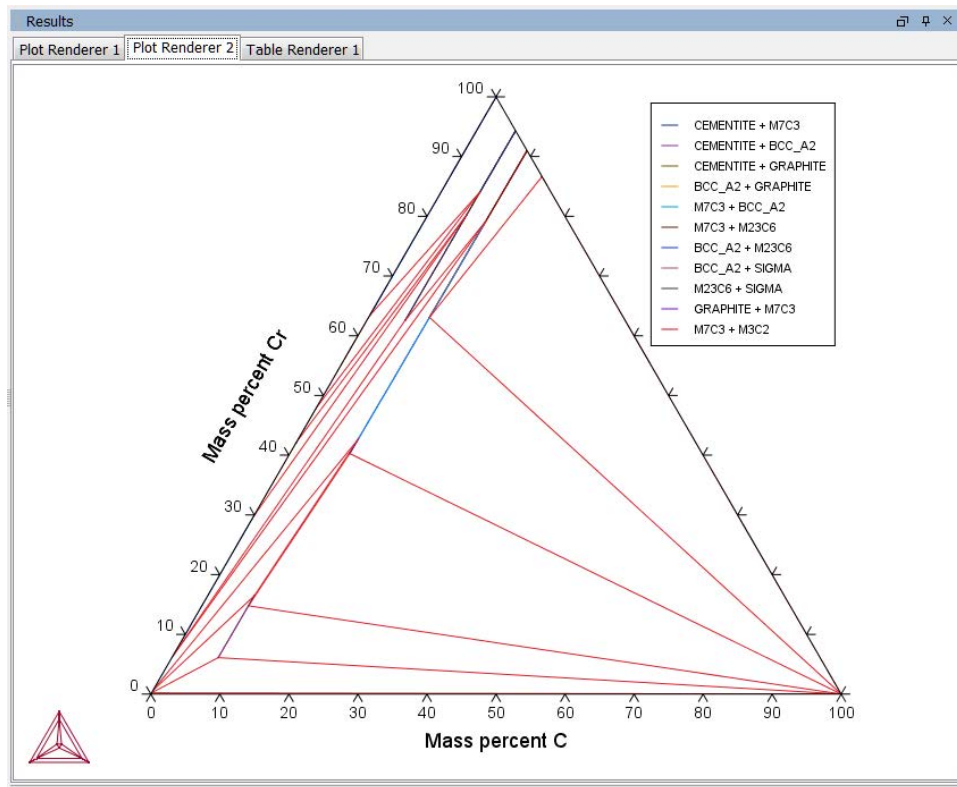
- add more than one Plot Renderer to its predecessor node (i.e. one of the calculator activities),
- add axes to the plots, and
- merge results in one plot.

PLOTS CAN HAVE MORE THAN ONE PREDECESSOR

A Plot Renderer can have several predecessors (if you want to plot several calculations in the same diagram), in which case there are several tabs in the Configuration window, one for each predecessor.

Several Plot Renderer activities (as well as Table Renderer activities) can be shown in the Results window as different tabs. The figure is from Graphical Mode example T_04.

▶ ["Plotting Several Calculations in One Diagram" on page 212](#)

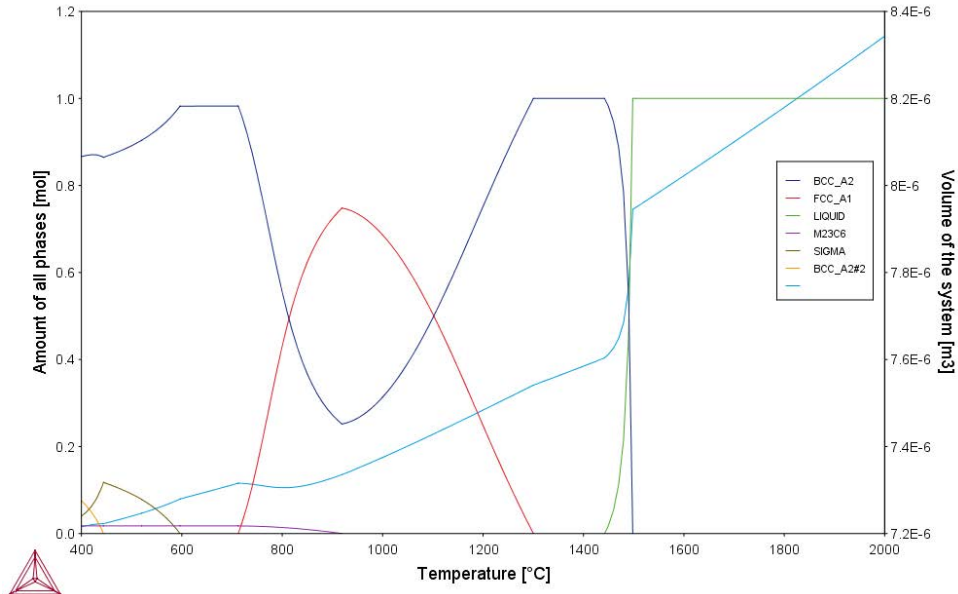


ADD AXES TO PLOTS

You can add additional X- and/or Y-axes to a plot to compare two or more variables at the same time as in the figure.

► ["Adding Axes to a Diagram" on page 216](#)

Two variables plotted on the Y-axis.



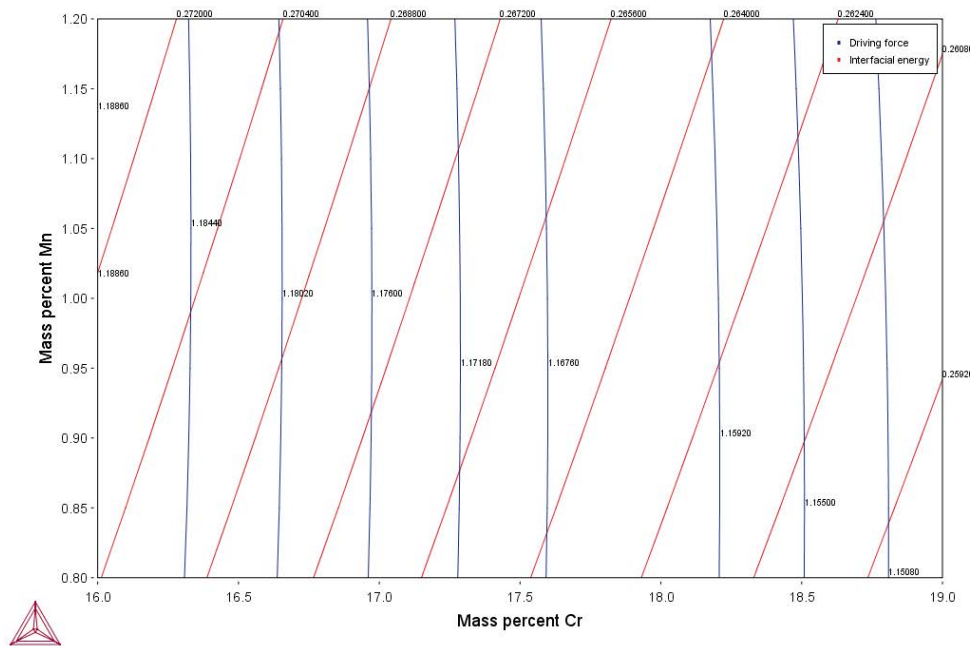
MERGE RESULTS IN ONE PLOT

You can merge (or overlay) calculated results for several variables into one plot. This is similar to adding an axis, but instead of displaying different variables along the X- and/or Y-axes, the same X and Y variables are used to compare the third variable (defined in the Plot Renderer as the Z-axis).

As in the figure (from example PM_G_03 in Graphical Mode Examples), the driving force and interfacial energy results are combined into one diagram. The X and Y axis is the same for both (Mass percent Cr/Mass percent Mn).

► ["Merging Plots into One Diagram" on page 214](#)

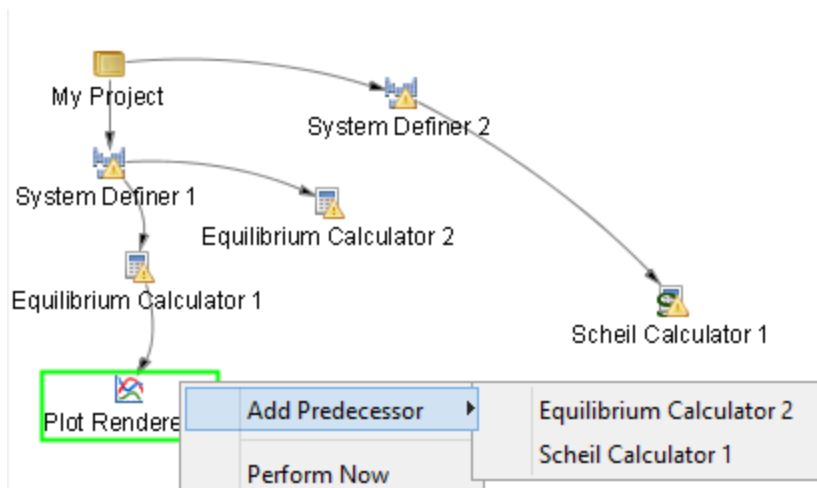
A contour plot showing both the driving force and interfacial energy calculation results comparing Mass percent Cr to Mass percent Mn.



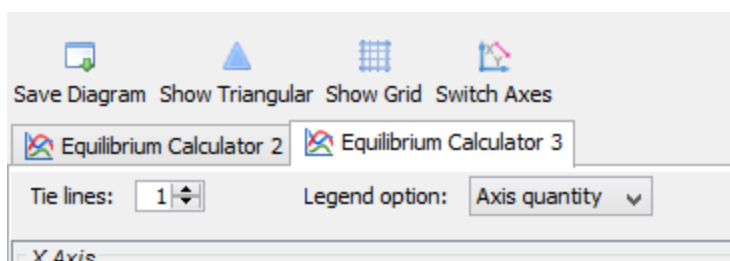
Plotting Several Calculations in One Diagram

To plot several calculations in one diagram, you must have, in addition to the Plot Renderer's original predecessor, at least one available Plot Renderer predecessor in your project, for example, the additional predecessor can be an Equilibrium Calculator, Binary Calculator, Ternary Calculator, Scheil Calculator or Experimental File Reader.

1. In the Project window click the **Plot Renderer** node.
2. In the **Configuration** window click **Add Predecessor**. Or right-click the **Plot Renderer** and choose **Add Predecessor**.

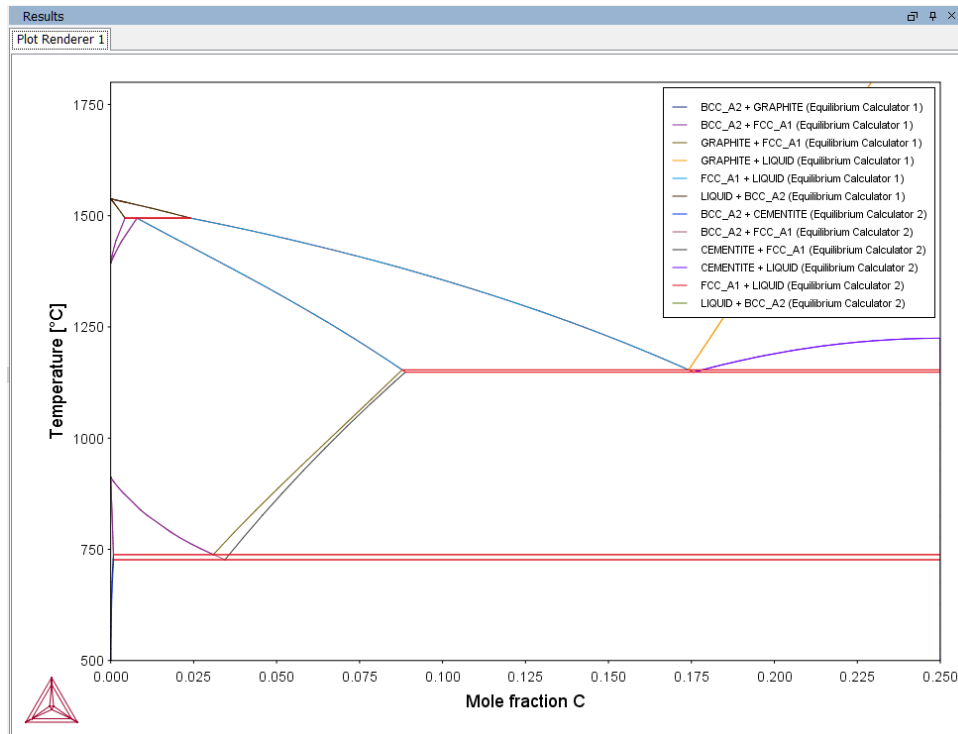


3. Select a predecessor. When added, the extra predecessor is linked to the Plot Renderer. On the Plot Renderer's Configuration window, the predecessors are shown as two tabs:



4. Configure how you want each calculation plotted on the tabs in the **Configuration** window, then click to **Perform** the Plot Renderer activity.

The calculations are plotted in the same diagram in a tab in the **Results** window. If any of the axis variables of the plots differ, then the label and scale of all calculations are shown parallel to each other. The following screen shot shows a diagram in which two calculations with different plotting axes variables have been plotted.



Merging Plots into One Diagram

You can merge (or overlay) calculated results for several variables into one diagram. The same X and Y variables are used to compare the third variable (defined in the Plot Renderer as the Z-axis).



You cannot overlay heat map or frequency plots.

The following uses example PM_G_03 in Graphical Mode Examples to describe the steps to overlay two plots: the driving force and interfacial energy results are combined into one diagram. The X and Y axis is the same for both (Mass percent Cr/Mass percent Mn).

1. In the **Project** window right-click the calculator node (e.g. Property Model Calculator) and add a **Plot Renderer** node from the **Create New Successor** menu.
2. Click the **Plot Renderer** node.
3. In the **Configuration** window, define the plot. Available settings are based on the calculation type.

EXAMPLE

In this example the Property Model Calculator is set to a *Grid* calculation type.

Choose **On** for the **Legend** option and **Contour** as the **Plot type**.

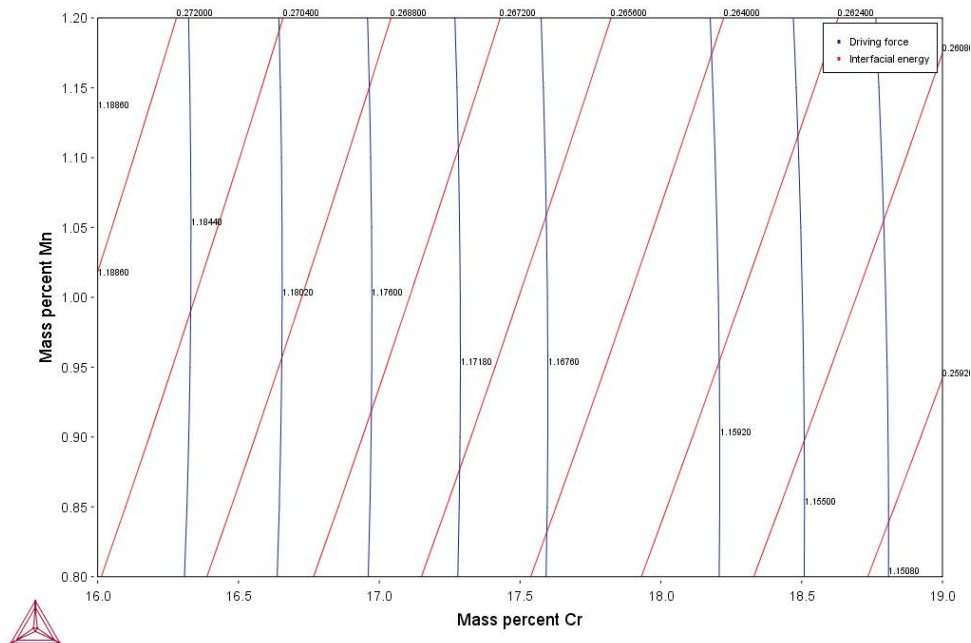
X Axis
 Axis variable: Mass percent Mn
 Axis type: Linear
 Limits: 0.0 to 100.0 step 10.0 ☒ Automatic scaling

Y Axis
 Axis variable: Temperature Celsius
 Axis type: Linear
 Limits: 500.0 to 3000.0 step 250.0 ☒ Automatic scaling

Z Axis
 Axis variable: Driving force
 Axis type: Interfacial energy
 Limits: 0.0 to 1.0 step 0.1 ☒ Automatic scaling


4. Click the **Add an axis** button. A new axes settings section is added underneath.
5. From the Z Axis section choose the **Axis variable**. In this example, **Interfacial energy**.
6. Click **Perform** to plot both on the same diagram.

In this case, a contour plot showing both the driving force and interfacial energy calculation results comparing Mass percent Cr to Mass percent Mn.

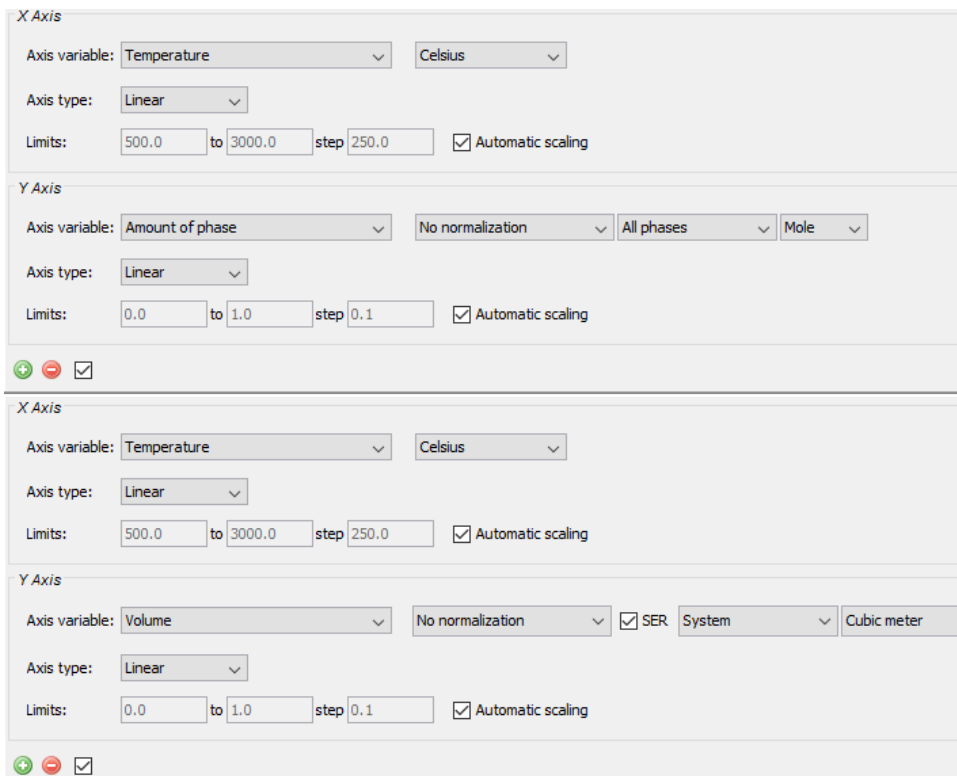


Adding Axes to a Diagram

You can add additional X- and/or Y-axes to a plot to compare two or more variables at the same time.

1. In the **Project** window right-click the calculator node (e.g. an Equilibrium Calculator) and add a **Plot Renderer** node from the **Create New Successor** menu.
2. Click the **Plot Renderer** node.
3. In the **Configuration** window, define the plot. Available settings are based on the calculation type.
4. Click the **Add an axis**  button. A new settings section is added underneath.
5. From the *X Axis* and/or *Y Axis* sections define another **Axis variable** and choose an **Axis type**.
6. Click **Perform** to plot both variables on the selected axis, in this example, the Y-axis.

In this example **Amount of phase** and **Volume** are selected as the Y-axis variables and **Temperature** as the X-axis variable. The plot is an example of the output.



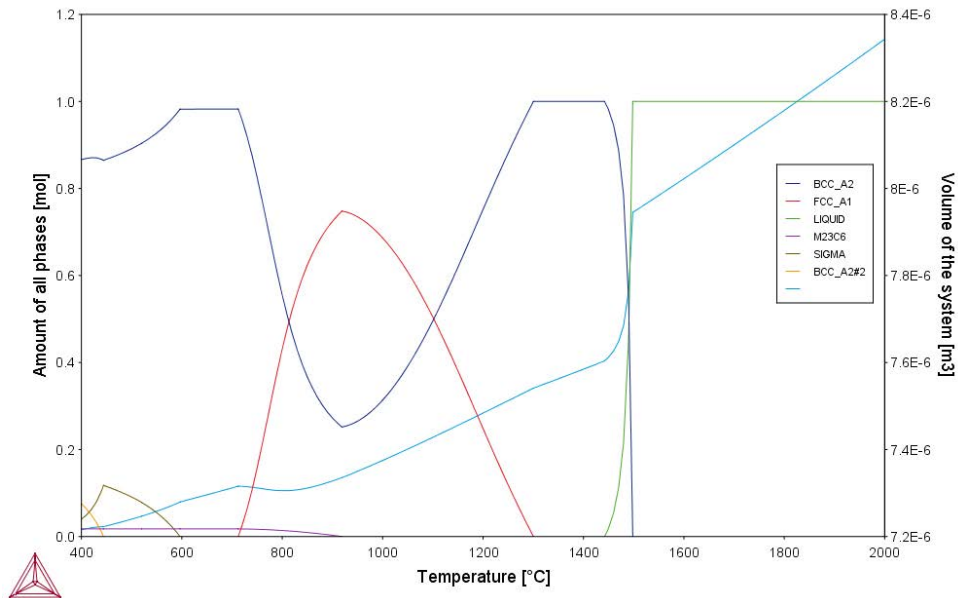
The image shows a configuration window for a plot with two identical sections for defining axes.

Section 1:

- X Axis:**
 - Axis variable: Temperature
 - Axis type: Linear
 - Limits: 500.0 to 3000.0 step 250.0
 - ☒ Automatic scaling
- Y Axis:**
 - Axis variable: Amount of phase
 - Axis type: Linear
 - Limits: 0.0 to 1.0 step 0.1
 - ☒ Automatic scaling

Section 2:

- X Axis:**
 - Axis variable: Temperature
 - Axis type: Linear
 - Limits: 500.0 to 3000.0 step 250.0
 - ☒ Automatic scaling
- Y Axis:**
 - Axis variable: Volume
 - Axis type: Linear
 - Limits: 0.0 to 1.0 step 0.1
 - ☒ Automatic scaling



Heat Map, Contour and 3D Plots

Grid Calculations

Using an Equilibrium, Property Model, or Process Metallurgy Calculator, you can choose to plot a *Heat map*, *Contour* or *3D* diagram.

- ▶ ["Equilibrium Calculator" on page 48](#), ["Property Model Calculator" on page 75](#), and ["Process Metallurgy Calculator" on page 163](#)

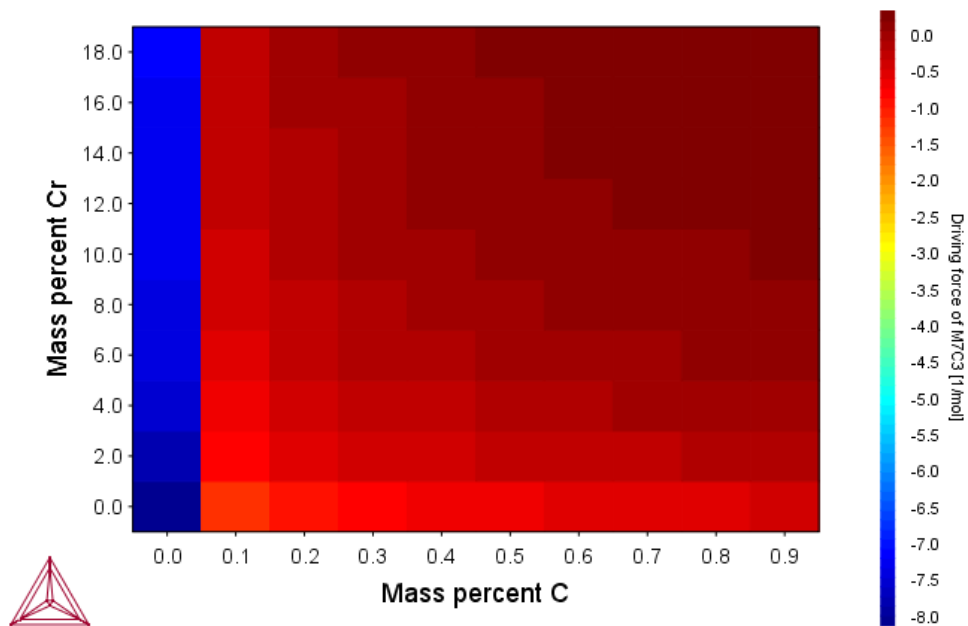
HEAT MAP

Each Z-axis variable value in the grid is represented by a color-coded area, where dark red represents the highest Z-axis variable value and dark blue represents the lowest Z-axis variable value.

Using an Equilibrium Calculator



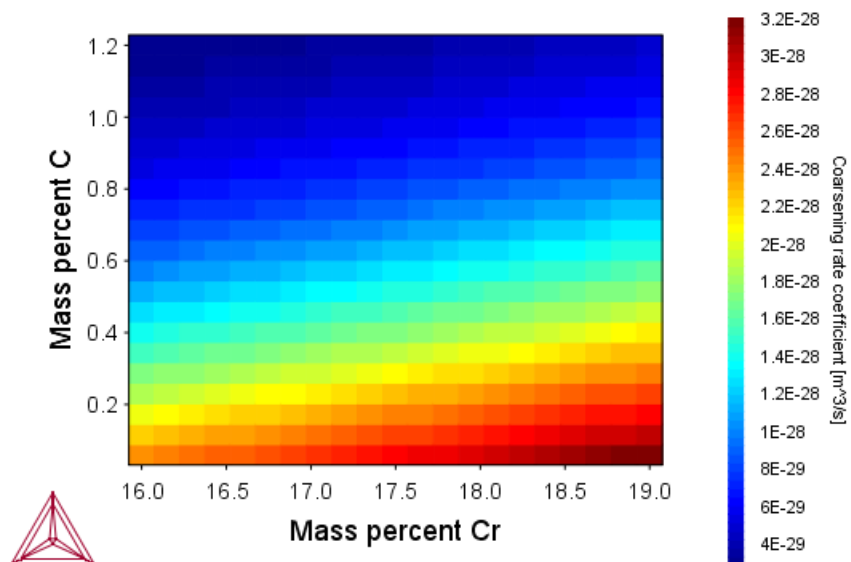
Equilibrium Calculator: ["T_09: Carbide Driving Force Heat Map" on page 262](#)



Using a Property Model Calculator



Property Model Calculator: ["PM_G_02: Coarsening and Interfacial Energy" on page 267](#)



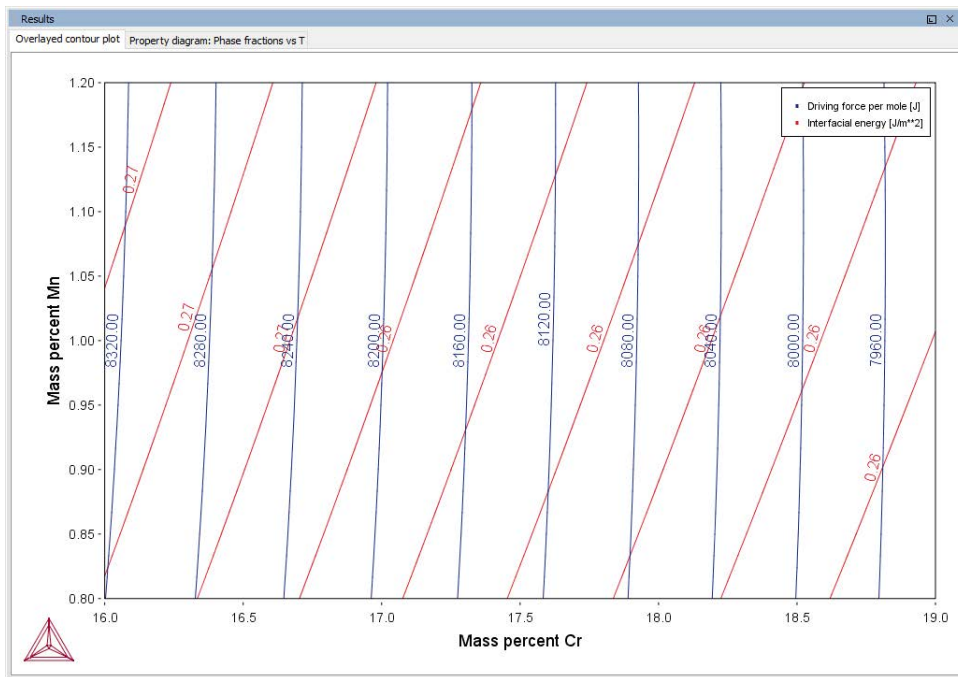
CONTOUR

Using a Property Model Calculator

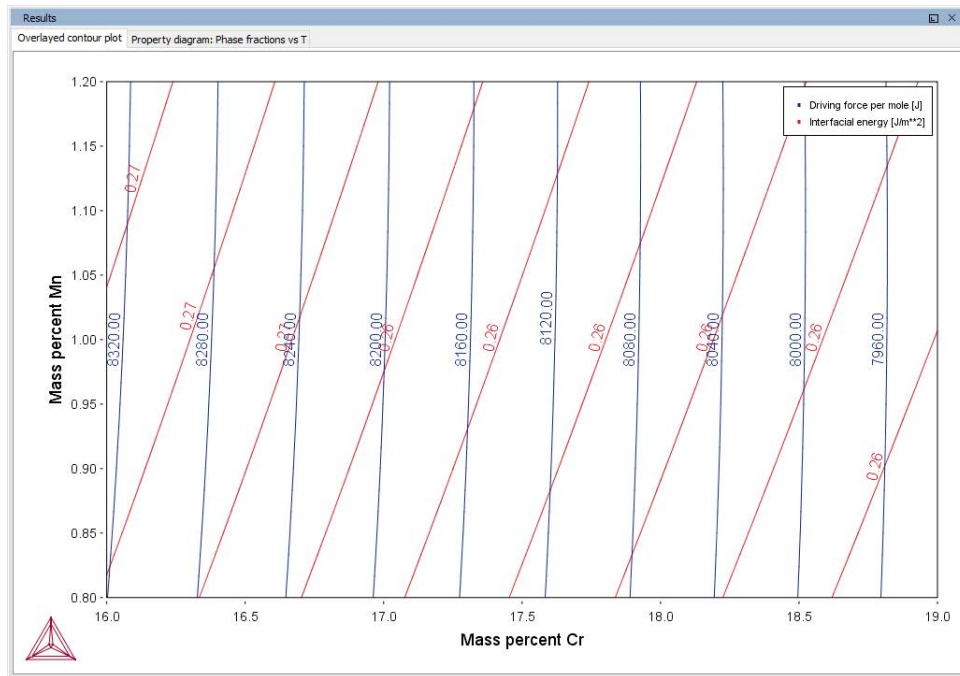


Property Model Calculator example: ["PM_G_03: Driving Force and Interfacial Energy" on page 271](#)

Z-axis variable values are traced with curves in the same way that height values are traced with curves on a topographical map. The colors used originate from the different data series.



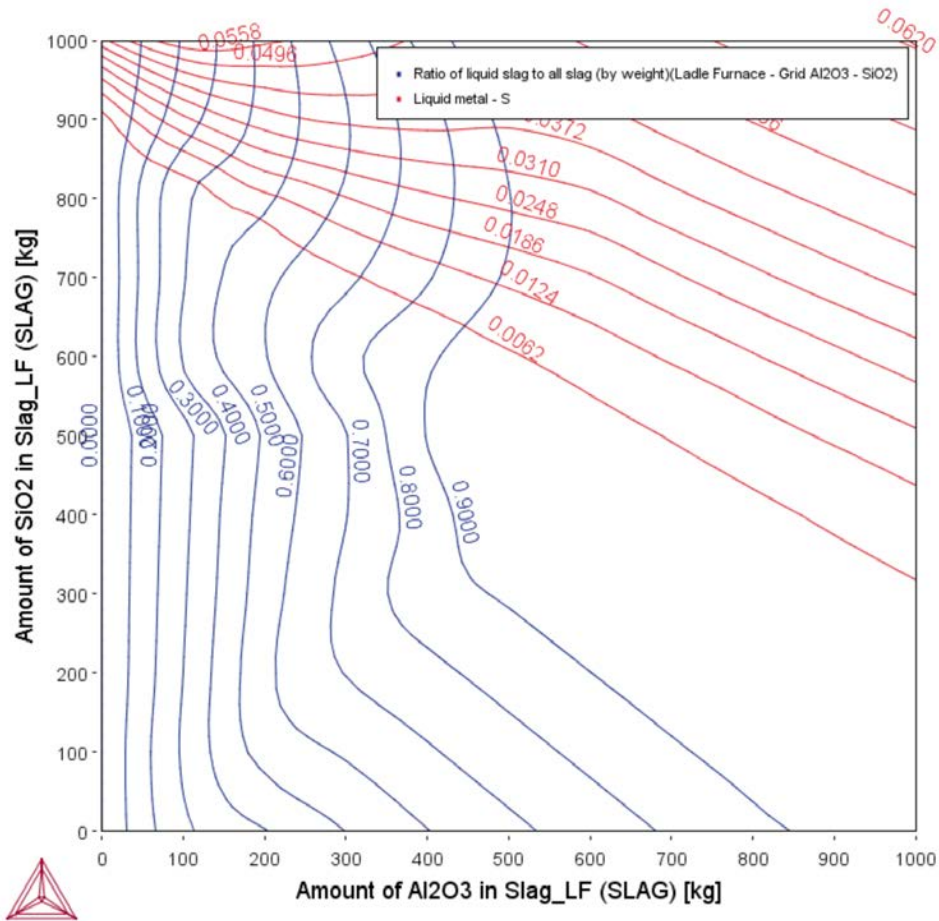
Z-axis variable values are traced with curves in the same way that height values are traced with curves on a topographical map. The colors used originate from the different data series.



Using a Process Metallurgy Calculator



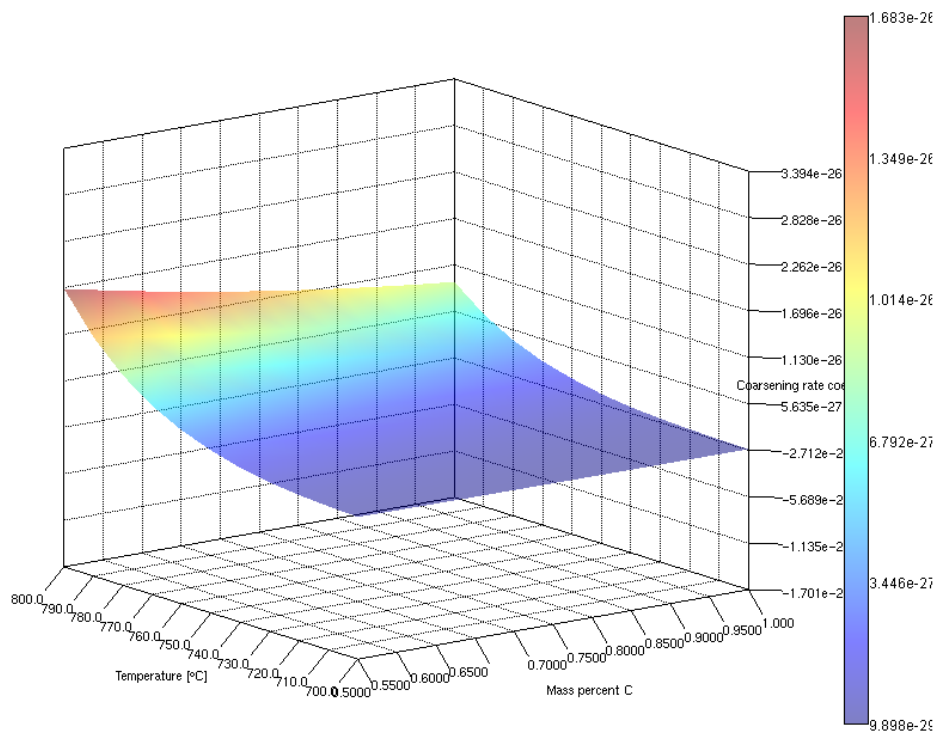
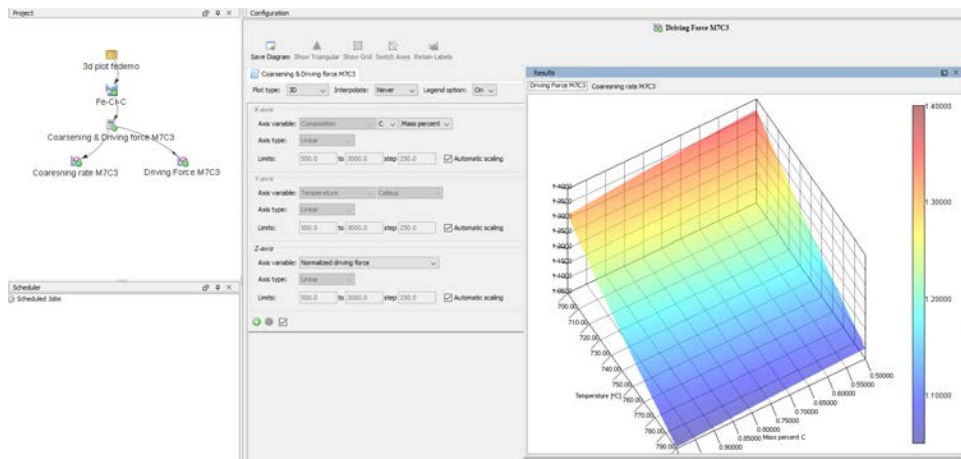
Process Metallurgy Calculator: ["PMET_02: Ladle Furnace" on page 294](#)



3D

► ["Rotating 3D Plots" on page 231](#)

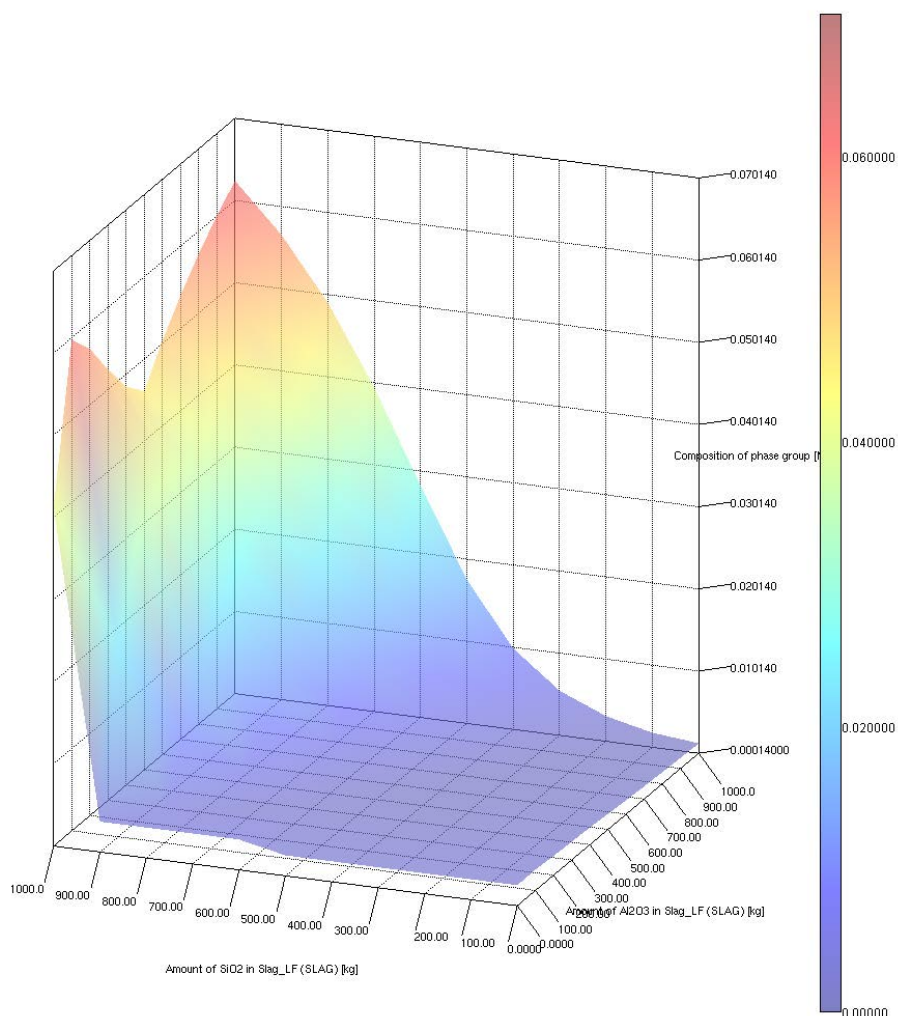
Using a Property Model Calculator



Using a Process Metallurgy Calculator



Process Metallurgy Calculator: ["PMET_02: Ladle Furnace" on page 294](#)



Note when detaching a Results window with a 3D plot

If you detach a **Results** window that contains a 3D plot, the screen may go black. To get the plot back simply regenerate it from the **Configuration** window (click **Perform** or **Perform Tree** at the bottom of the window).

Note for Linux OS Using VirtualBox

The following is applicable to users running Thermo-Calc under Linux in a virtual machine using VirtualBox.

Due to limitations in the OpenGL-drivers for VirtualBox, you will experience problems with 3D-plots unless the 3D-acceleration is disabled for the virtual machine being used.

To disable the 3D-acceleration:

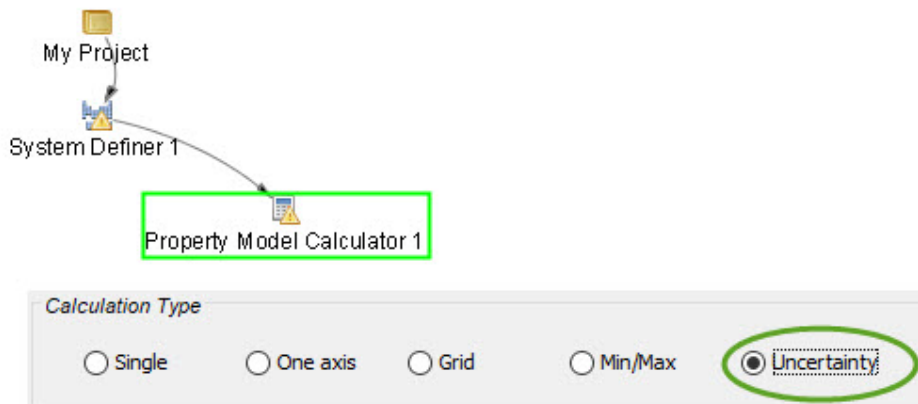
1. Open the main VirtualBox application.
2. In the list, right-click on the virtual machine running Thermo-Calc.
3. Select **Settings**.
4. Navigate to **Display**.
5. On the **Screen** tab, click to clear the **Enable 3D acceleration** check box.



If you are using other virtualization software and experience problems with the 3D plot, a similar solution might apply.

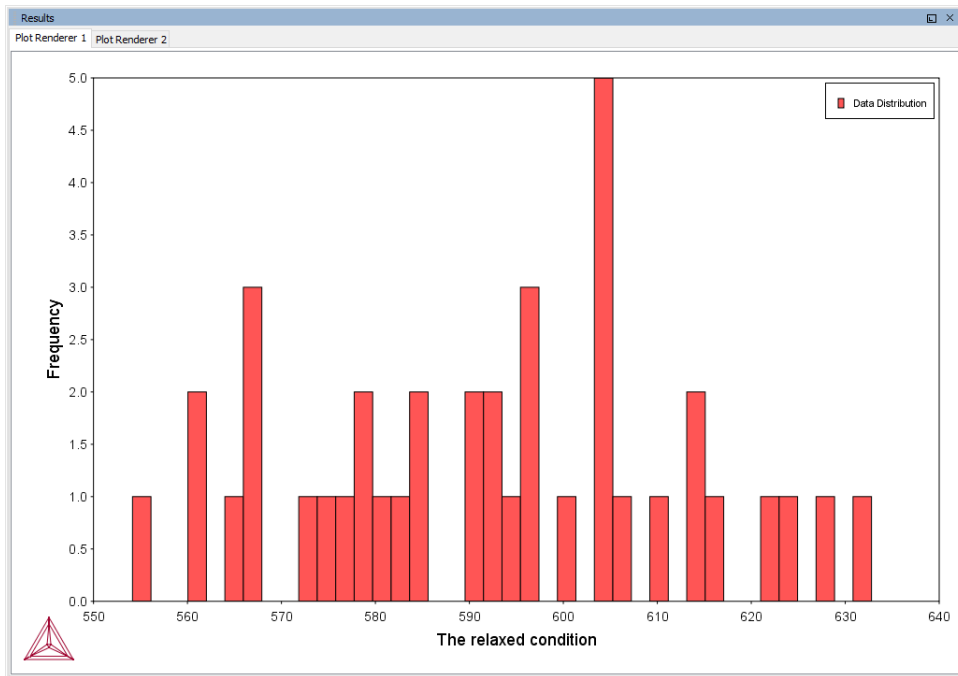
Uncertainty Calculations

Using a **Property Model Calculator** or **Process Metallurgy Calculator** (Uncertainty calculation) you can choose to create either a *histogram* or *probability* plot.

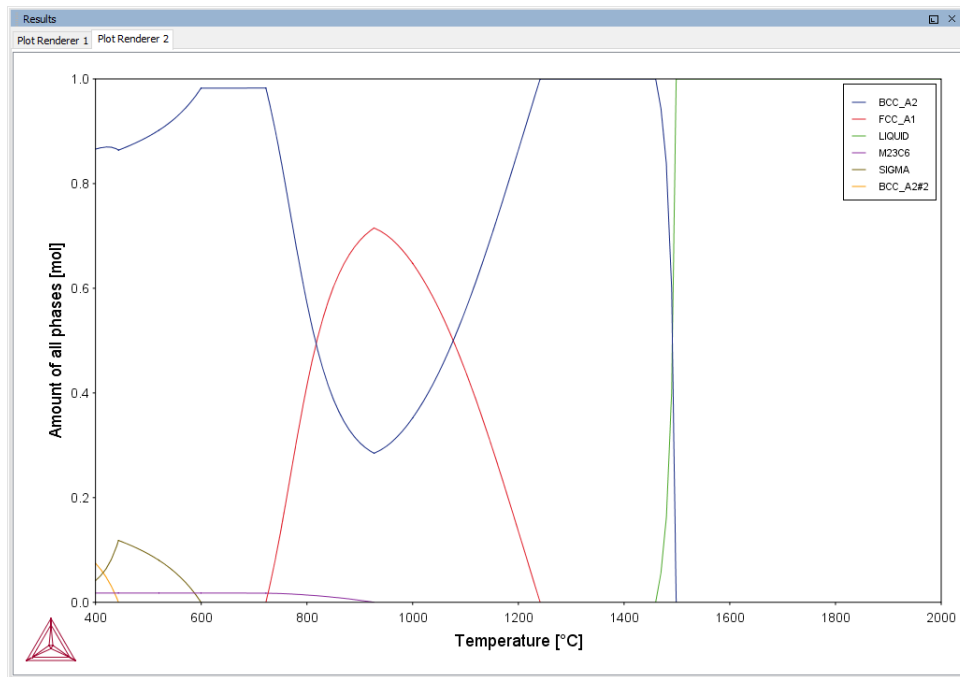


The following use the Property Model Calculator example: ["PM_G_01: Phase Transition" on page 265](#)

HISTOGRAM



PROBABILITY



About the Uncertainty Calculations

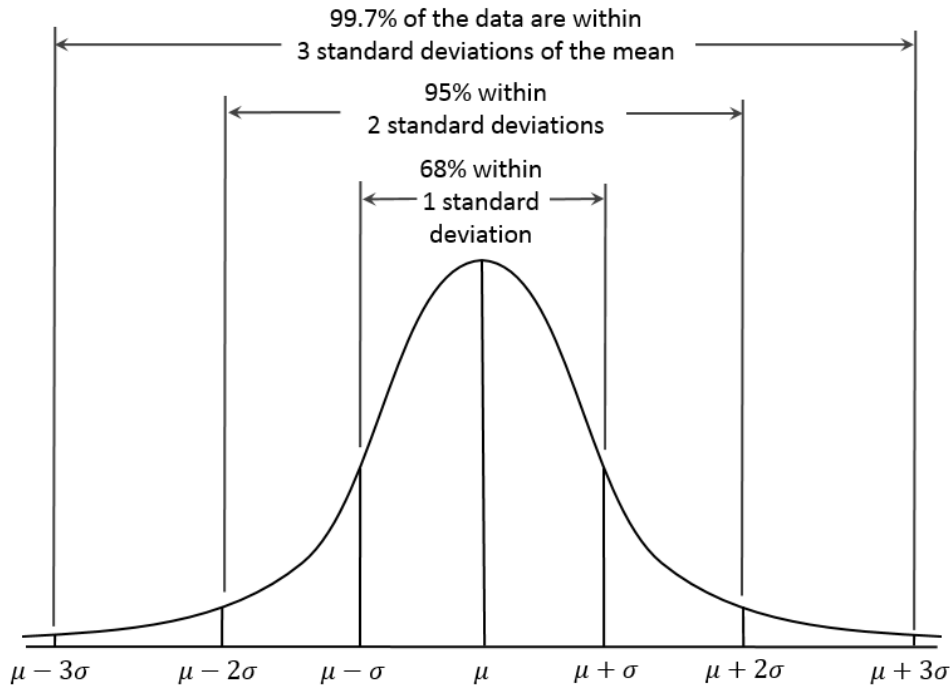
The **Uncertainty** calculation in Thermo-Calc uses the values (the mean) entered for quantities in the Condition Definitions section as the starting point to estimate, within a certain probability, the true variation of the quantity. Uncertainty calculations are available with the Property Model Calculator and the Process Metallurgy Calculator.

An example of a Gaussian distribution is shown next. The example uses the ["Phase Transition Model" on page 83](#) and an **Uncertainty Calculation Type** to describe how the sampling of data is performed. The example ["PM_G_01: Phase Transition" on page 265](#) predicts the transition temperature to the unwanted brittle Sigma phase and shows how the temperature is influenced by changes to a steel alloy's composition.

GAUSSIAN DISTRIBUTION, THE 3-SIGMA RULE

- The *mean* is at the peak of the curve (labeled μ).
- The *standard deviation* (σ) is a plus and minus range, $\pm 1\sigma$, $\pm 2\sigma$ or $\pm 3\sigma$, of the variance from the mean.

Image by Dan Kernler: https://en.wikipedia.org/wiki/Normal_distribution#/media/File:Empirical_Rule.PNG.



As long as the number of events (the sample size) is very large, then the Gaussian distribution function can be used to describe physical events. A Gaussian distribution is assumed to describe how each quantity varies in an uncertainty calculation, as shown next.

CONDITION DEFINITIONS AND SAMPLING SETTINGS

In Thermo-Calc, the mean of the quantity's distribution is defined in the *Condition Definitions* section. The **Mean** is then used in the *Sampling of Data from Gaussian Distributions* section as the starting point for how much you want to deviate from this value.

The mean defined in Condition Definitions is used during the sampling.

Composition unit Mass percent

Condition Definitions

| | | |
|-------------|----------------------|------------------------------------|
| Temperature | Celsius | <input type="text" value="600.0"/> |
| Composition | Fe | <input type="text" value="80.52"/> |
| Composition | Ni | <input type="text" value="1.4"/> |
| Composition | C | <input type="text" value="0.08"/> |
| Composition | Mn | <input type="text" value="1.0"/> |
| Composition | Cr | <input type="text" value="17.0"/> |

Sampling of Data from Gaussian Distributions

| Quantity | Mean | Δ Min/Max |
|-----------------------------------------------------|------------------------------------|-----------------------------------|
| <input type="checkbox"/> Temperature | <input type="text" value="600.0"/> | <input type="text" value="0.0"/> |
| <input checked="" type="checkbox"/> Mass percent Ni | <input type="text" value="1.4"/> | <input type="text" value="0.4"/> |
| <input checked="" type="checkbox"/> Mass percent C | <input type="text" value="0.08"/> | <input type="text" value="0.02"/> |
| <input checked="" type="checkbox"/> Mass percent Mn | <input type="text" value="1.0"/> | <input type="text" value="0.3"/> |

The values entered in the Δ **Min/Max** fields are the resulting width of the distribution corresponding to the 95% confidence interval (approximately $\mu \pm 2\sigma$) shown in *Gaussian distribution, the 3-sigma rule*. This confidence interval means that approximately 95% of the sampled values fall within these limits, as shown next.

SAMPLING PARAMETER SETTINGS

The default value for truncating the distribution is set at **3 standard deviations** in the *Sampling Parameters* section. This is also where you set the **Total number of samples**. The default is 200. In order to maintain a Gaussian distribution for the varied quantities, this number should not be too low.

Sampling Parameters

Truncate distribution at standard deviations

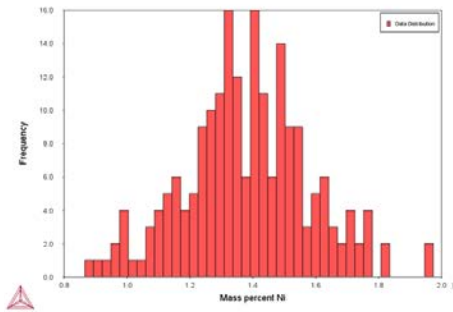
Total number of samples

You can experiment by varying the conditions and the number of samples to see the distribution results smooth out as is to be expected based on the Central Limit Theorem, as shown in the histogram plot. You can also plot the results as a normal probability.

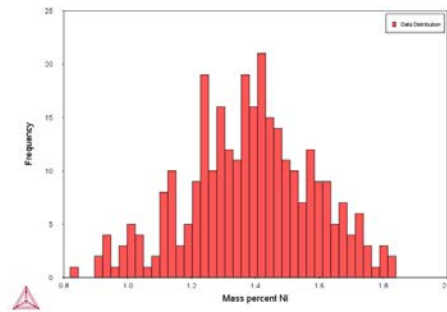
HISTOGRAM PLOT

This series of histogram plots shows the uncertainty calculations sampling data from Gaussian distributions. On the **Plot Renderer** the variable is set to measure the **Composition** of **Ni**. It compares the Ni composition where the total sample size is increased. In the example, the initial sample size uses the default, 200, and then the sample size is increased to 300, 400, 600, 800, and 1000, showing how the plot follows the Gauss distribution.

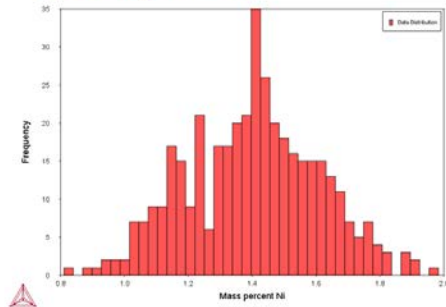
Total samples = 200



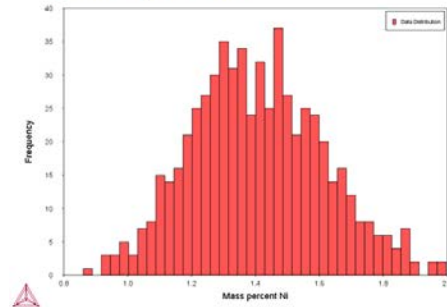
Total samples = 300



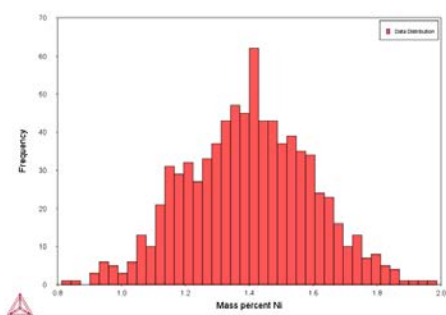
Total samples = 400



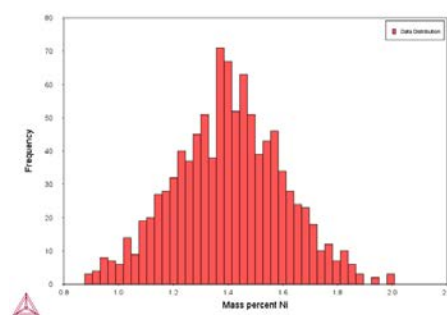
Total samples = 600



Total samples = 800



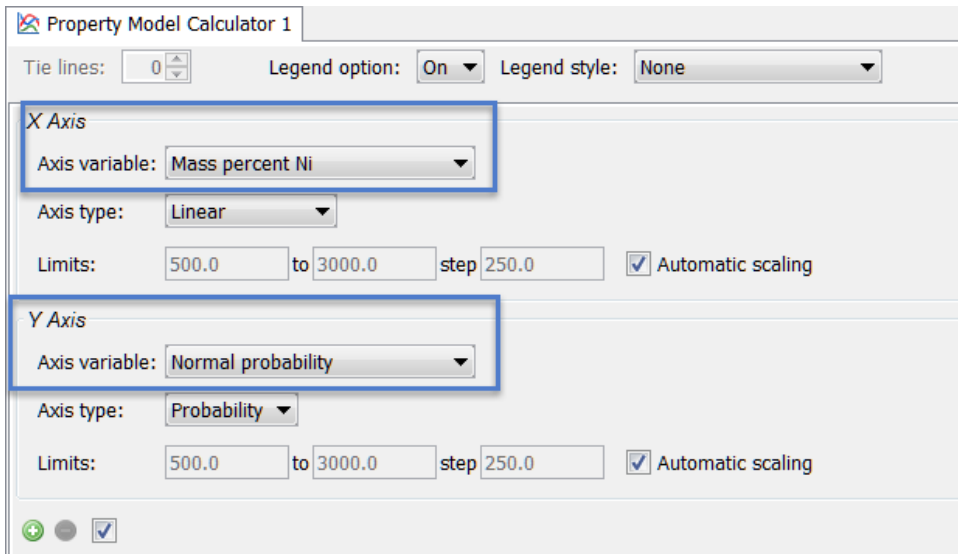
Total samples = 1000



NORMAL PROBABILITY PLOT

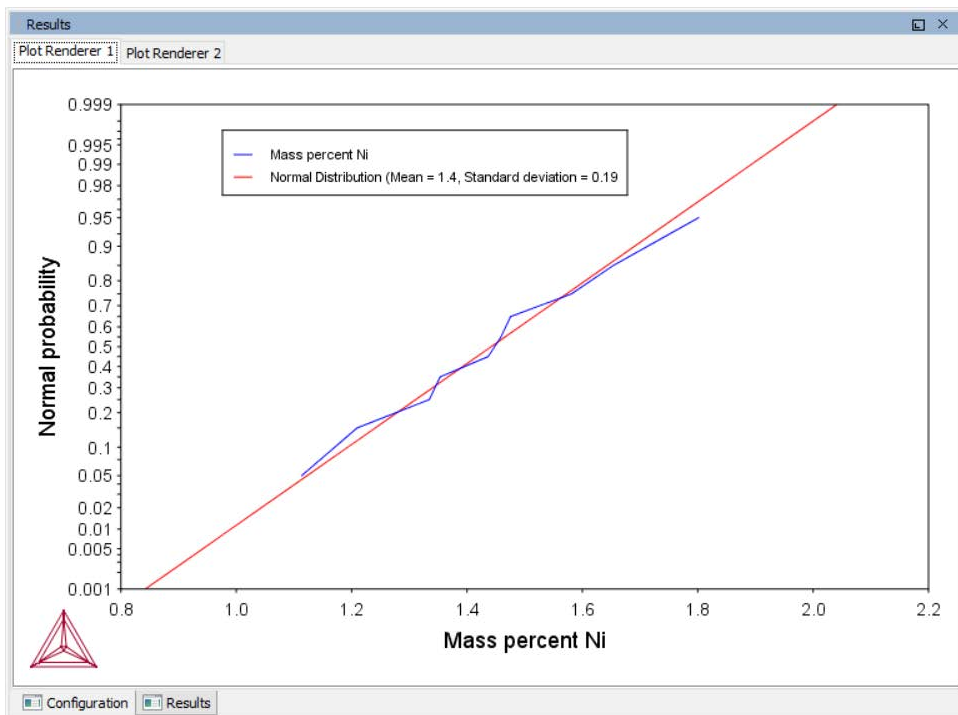
You can also plot the results as a Normal probability. Continuing with this example, on the

Property Model Calculator Configuration window the X-Axis variable is plotted as Composition and the Y-Axis variable is plotted as the Normal probability.



The image shows the 'Property Model Calculator 1' configuration window. At the top, there are settings for 'Tie lines' (0), 'Legend option' (On), and 'Legend style' (None). Below this, the 'X Axis' section is highlighted with a blue box. It contains 'Axis variable' set to 'Mass percent Ni', 'Axis type' set to 'Linear', and 'Limits' from 500.0 to 3000.0 with a step of 250.0. The 'Automatic scaling' checkbox is checked. Below the X Axis section, the 'Y Axis' section is also highlighted with a blue box. It contains 'Axis variable' set to 'Normal probability', 'Axis type' set to 'Probability', and 'Limits' from 500.0 to 3000.0 with a step of 250.0. The 'Automatic scaling' checkbox is also checked. At the bottom left, there are three small icons: a green plus, a grey circle, and a blue checkmark.

This is a normal probability plot example of the uncertainty calculations sampling data from Gaussian distributions. It compares the Ni composition where the total sample size is 200. The sampled data (blue line) closely follows the ideal normal distribution (red line). Deviations are naturally larger at the tails ($\approx 1\%Ni$ and $\approx 2\%Ni$) since the number of samples are fewer there compared to the center of the distribution.



Rotating 3D Plots

▶ ["Heat Map, Contour and 3D Plots" on page 217](#)

When you use a *Grid* calculation type you can plot the diagram in 3D.

In the **Results** window after you create the 3D plot:

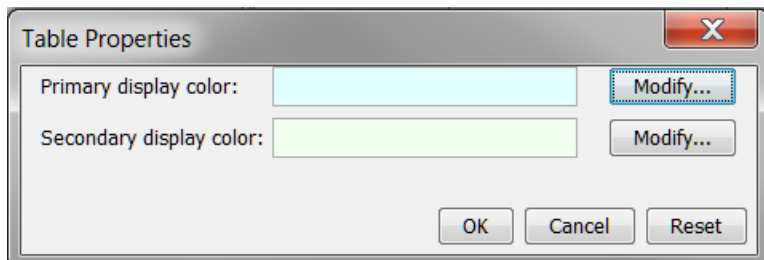
- Rotate the diagram automatically. Double-click in the **Results** window and the diagram rotates clockwise. Click once to stop the automatic rotation.
- Rotate the diagram manually. Click and hold the mouse and move it around the **Results** window.
- Use the mouse wheel to zoom in and out. To reset the plot to its default view click **Perform Tree** to regenerate the plot.

Plot and Table Formatting

In this section:

Setting Background Colours

To change the background colours of the table, in the **Results** window right-click a Table Renderer tab, and select **Properties**. Modify as required.



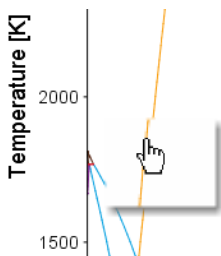
The defaults for these settings can be changed globally. To open the Options window: From the main menu select **Tools** → **Options** and click the **Activities** tab. Then click **Tabulation**.

Changing the Plot Properties

For global changes to the default settings plots see ["Global Settings: Graphical and Console Mode Plotting" on page 47](#). The settings are the same but applied to all new plots.

To make local changes to the appearance of a specific plot, in the **Results** window right-click a plot and select **Properties**. You can also edit some properties for individual plot lines (the color, the line width and type, and whether data points are included).

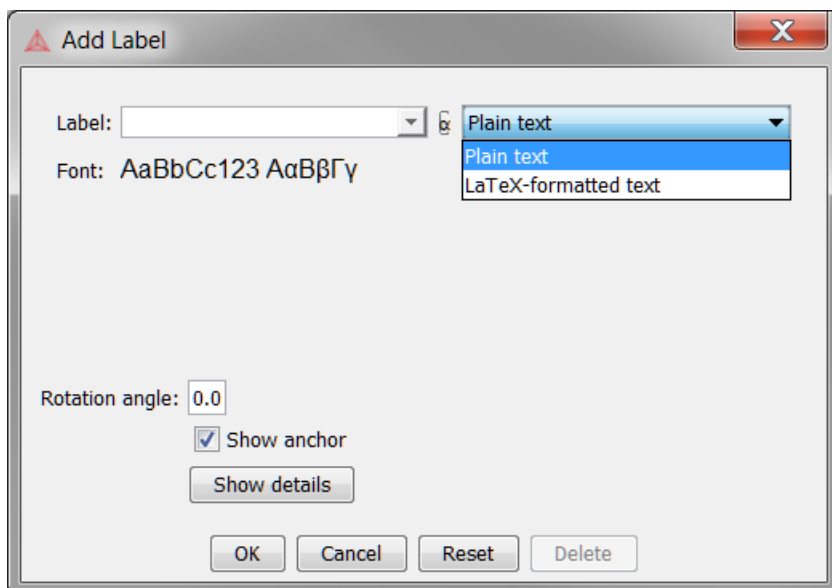
In the **Results** window, hover the mouse over a plot line. When it is over a line that can be clicked the crosshair cursor turns into a pointing finger.



To prevent unintended edits, hold down <Ctrl> while moving the cursor around the plot to only display it as a crosshair.

Plot Labels

To add a label text at a certain point in a plot, right click the point, and select **Add Label**. For phase diagrams, the program suggests a label that you can keep or edit. The suggested label specifies the names of the stable phases at the coordinate where you clicked. For all other plot types, you enter your own text, which can either be Plain text or LaTeX formatted text.



You can enter the label as **Plain text** or in **LaTeX-formatted text**. For **LaTeX-formatted text** enter or edit the text as required. For example, underscores (`_`) are added before the numbers to make subscripts in the label.



For a list of supported LaTeX commands, see:

<http://www2.ph.ed.ac.uk/snuggletex/documentation/math-mode.html>.

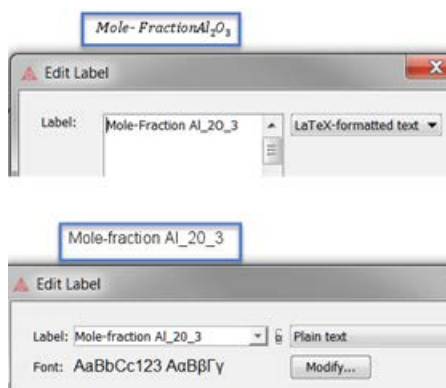


By default when using LaTeX, you are in math mode and Thermo-Calc automatically interprets the entered text as math. The above link uses the dollar sign (\$) in all the examples but this is NOT required. For example, if you enter `$E=mc^2$` this is displayed including the \$ instead of the equation.

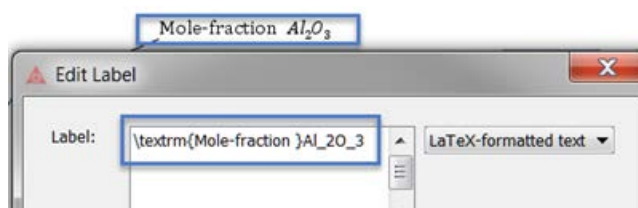
Plot Labels: Entering a Mixture of Plain Text and Equations

When you enter text using LaTeX formatted text it displays by default on the plot in italics and treats the text as an equation.

As in the following example, the top label does not display correctly because the label is a mixture of text (Mole-Fraction) and an equation (Al_2O_3). In the bottom image, when the same information is added as Plain text to the plot it now does not include the subscripts.



To add a mixture of plain text and equation text, you can exit math mode using the string `\textrm` followed by the text to display enclosed in curly brackets. For example `\textrm {Mole-fraction }Al_2O_3` results in the label as shown:



In this example, you need to add a space at the end of fraction in order to separate the text from the equation part of the label.



When working in Console Mode, you can also use the above windows on the Console Results window to add and edit labels. In addition, you can use the command.

Plot Labels: Rotation Angle and Show Anchor

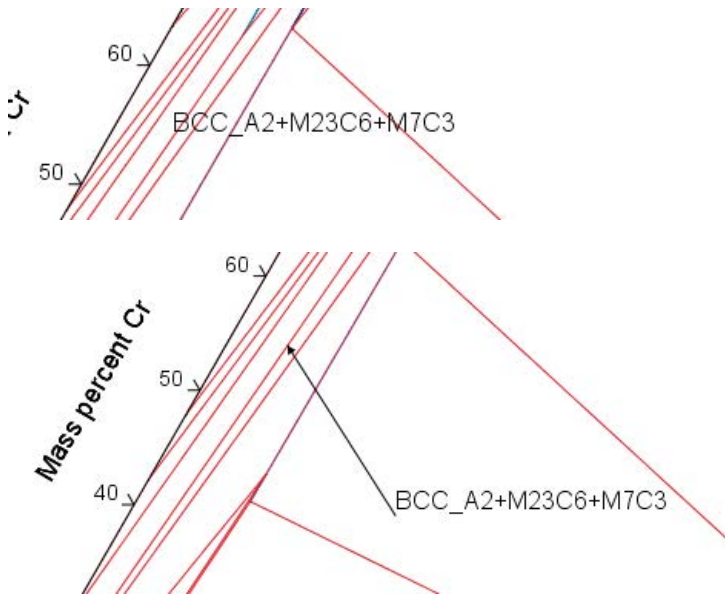
By default the **Show anchor** check box is selected, which includes an arrow from the label point to the coordinates.

If you do not want the label oriented horizontally in the Plot Renderer tab, then specify the number of degrees of rotation in the **Rotation angle** field.

Click **OK** to add the label to the plot. You can also move a label by clicking and dragging it. The default anchor arrow is added to indicate the point that belongs to the label.

Moving Plot Labels

Drag and drop labels anywhere on the plot. The anchor arrow points to the point of origin.



About Legend Styles

There are a variety of legend styles you can use to display detail about the phases. The same legend styles are available for both Graphical Mode and Console Mode plots.



For Console Mode, use the command `CHANGE_LEGEND`.

In Graphical Mode the label styles are defined when using the ["Plot Renderer" on page 179](#). You can select a **Legend style** for the **Stable phases** or **Axis quantity** selected for **Legend option**.

When there is a legend in the diagram you can append constitution and/or ordering descriptions to the phase name.

If constituent description is included in the legend, then for each equilibria along a line in the diagram, the largest constituent fractions are summed until they are equal or greater than 0.6. This is done separately for each sublattice. If the equilibria along the line gets different sets of constituents these are all appended to the list for that sublattice.

The ordering description is only printed for partitioned phases (phases that have a disordered contribution) that begins with at least two identical sublattices (sublattices where the set of constituents are identical). `DISORD` (disordered) is shown if site fractions are identical between identical constituents on all identical sub lattices (with an error margin) otherwise `ORD` (ordered) is shown in the legend.

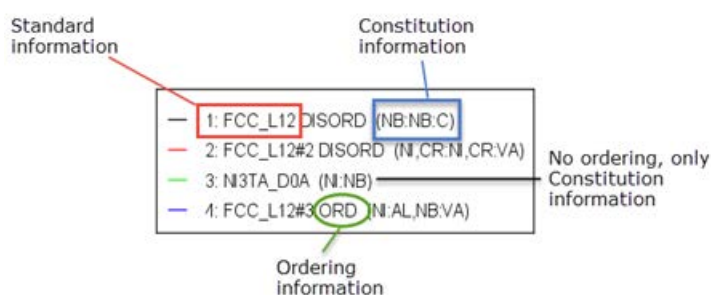
If ordering between equilibria in a line are different, then `ORD + DISORD` is shown in the legend.

Legend and Label Styles

Legend Styles

To show the differences between labels, the following uses the same example file that creates Figure 6 in TCNI database extended information document (found on the Thermo-Calc [website](#)).

When **All** is selected for this specific example the label includes the following:



Specifically:

- There are two disordered FCC phases (matrix and carbide), one ordered FCC (gamma prime), plus a phase NI3TA_D0A (called Delta in Ni-alloys).
- ORDERING shows the different FCC phases.
- CONSTITUTION shows that FCC_L12#1 is NbC, FCC_L12#2 is matrix with Ni and Cr as major constituent, FCC_L12#3 is Ni3Al with Nb addition and NI3TA_D0A is Nb-rich (eg. Ni3Nb).

Label Styles

These examples are for each label style choice - **None**, **All**, **Constitution** or **Ordering**. The instructions are for when you are setting the options using the Plot Renderer. In Console Mode, you choose the options (`ALL`, `NONE`, `CONSTITUTION`, or `ORDERING`) after the command `CHANGE_LEGEND`.

NONE

When **None** is selected the legend includes the standard information about the phases.

-
- 1: FCC_L12
 - 2: FCC_L12#2
 - 3: N3TA_D0A
 - 4: FCC_L12#3

ALL

When you select **All** the **Constitution description** and the **Ordering description** (when there is ordering) are included.

- 1: FCC_L12 DISORD (NB:NB:C)
- 2: FCC_L12#2 DISORD (N:CR:N:CR:VA)
- 3: N3TA_D0A (N:NB)
- 4: FCC_L12#3 ORD (N:AL:NB:VA)

CONSTITUTION DESCRIPTION

When you select **Constitution description**, this is added to the standard description.

- 1: FCC_L12(NB:NB:C)
- 2: FCC_L12#2(N:CR:N:CR:VA)
- 3: N3TA_D0A(N:NB)
- 4: FCC_L12#3(N:AL:NB:VA)

ORDERING DESCRIPTION

When you select **Ordering description** and when there is ordering, this is added to the standard description.

- 1: FCC_L12 DISORD
- 2: FCC_L12#2 DISORD
- 3: N3TA_D0A
- 4: FCC_L12#3 ORD

Graphical Mode Examples

► ["About the Examples " on page 23](#)

This guide includes descriptions of the following examples.

| Category | Example number |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------|
| "Thermo-Calc Graphical Mode Examples Collection" on the next page includes binary and ternary system examples, Scheil, the Equilibrium Calculator, plus more | T_01 to T_10 |
| "Thermo-Calc Property Model Examples Collection" on page 265 : General and Steel models | General models: PM_G_01 to PM_G_06 Steel models: PM_Fe_01 to PM_Fe_03 |
| "Process Metallurgy Examples Collection" on page 288 | PMET_01 to PMET_03 |
| "Diffusion Module (DICTRA) Graphical Mode Examples" on page 308 | D_01, D_02, D_03 (the Quick Start Guide Examples) D_04 to D_07 |
| "Precipitation Module (TC-PRISMA) Graphical Mode Examples" on page 330 | P_01 to P_13 |

Thermo-Calc Graphical Mode Examples Collection

T_01: Calculating a Single-Point Equilibrium

This example shows the result from a single-point equilibrium calculation in the Fe-C system. It demonstrates the use of the Equilibrium Calculator and generates a Table Renderer in the **Results** window. The number of equilibrium conditions is $C+2$ where C is the number of components, meaning that four conditions are needed in this example:

- **Temperature** is 1000 K
- **Pressure** is 101325 Pa
- **System size** is 1 mole
- **Mass percent carbon** is 0.1%

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

- Folder: Thermo-Calc
- File name: *T_01_Single-point_equilibrium.tcu*



This example is included as a tutorial on our [website](#) and our [YouTube](#) channel.

TABLE RESULT

The displayed results of the calculation show that the BCC_A2 (ferrite) and GRAPHITE phases are stable for this set of equilibrium conditions.

| Results | | | | |
|----------------------|----------------------|----------------------|------------------------|------------------|
| Table Renderer 1 | | | | |
| System | | | | |
| Moles | 1.00000 | | | |
| Mass | 55.64392 | [g] | | |
| Temperature | 1000.00000 | [K] | | |
| Total Gibbs Energy | -42141.28527 | [J] | | |
| Enthalpy | 24706.54116 | [J] | | |
| Volume | 7.30619E-6 | [m3] | | |
| <i>Component</i> | <i>Mole Fraction</i> | <i>Mass Fraction</i> | <i>Activity</i> | <i>Potential</i> |
| C | 0.00463 | 0.00100 | 0.21816 | -12658.89428 |
| Fe | 0.99537 | 0.99900 | 0.00619 | -42278.50542 |
| Stable Phases | | | | |
| | <i>Moles</i> | <i>Mass</i> | <i>Volume Fraction</i> | |
| BCC_A2#1 | 0.99609 | 55.59692 | 0.99711 | Composition ▾ |
| Composition | | | | |
| <i>Component</i> | <i>Mole Fraction</i> | <i>Mass Fraction</i> | | |
| Fe | 0.99928 | 0.99984 | | |
| C | 0.00072 | 0.00016 | | |
| | <i>Moles</i> | <i>Mass</i> | <i>Volume Fraction</i> | |
| GRAPHITE#1 | 0.00391 | 0.04700 | 0.00289 | Composition ▾ |
| Composition | | | | |
| <i>Component</i> | <i>Mole Fraction</i> | <i>Mass Fraction</i> | | |
| C | 1.00000 | 1.00000 | | |
| Fe | 0.00000 | 0.00000 | | |

T_02: Stepping in Temperature in the Fe-C System

This example shows how the fractions of stable phases vary for an Fe-0.1 mass-% C alloy when the temperature is varied between 500 and 2000 K. It demonstrates the use of the Equilibrium Calculator. To allow temperature to vary, the corresponding **Axis Definition** check box is selected.

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

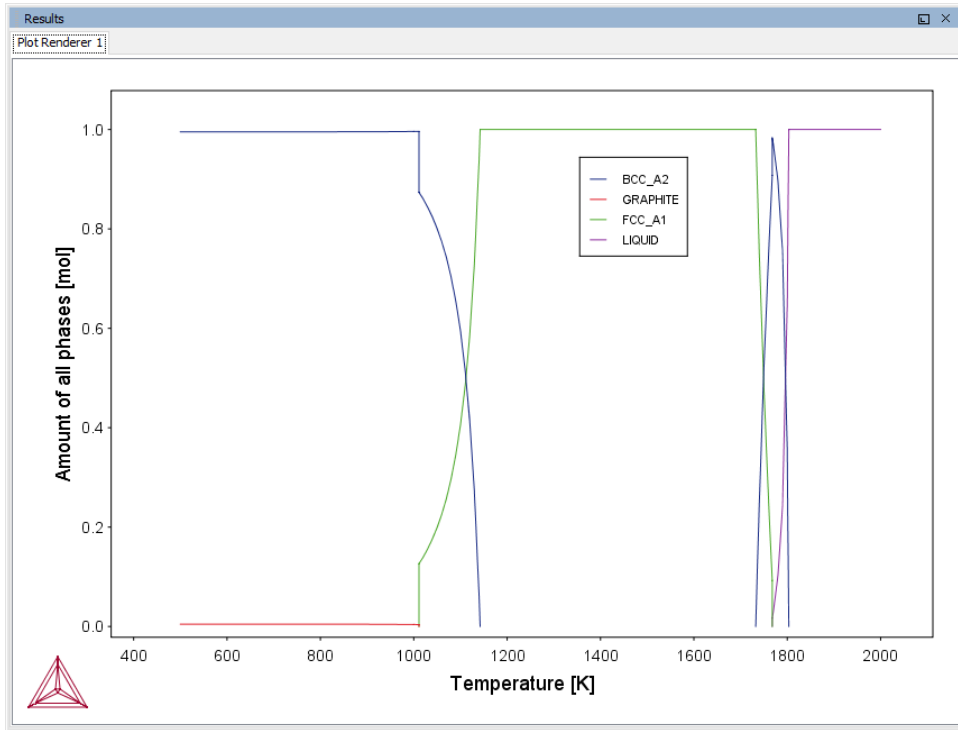
- Folder: Thermo-Calc
- File name: *T_02_Step_in_temperature_in_Fe-C.tcu*



This example is included in the tutorial on our [website](#) and [YouTube](#) channel.

PLOT RESULT

In this example, results are displayed graphically using a Plot Renderer activity.



If you want, you can use a Table Renderer to generate text results instead, as shown in this example after adding a Table Renderer to the Equilibrium Calculator and clicking **Perform**.

| Results | | | | |
|-----------------|------------------------|------------------------|--------------------------|------------------------|
| Plot Renderer 1 | | Table Renderer 1 | | |
| Temperature [K] | Amount of BCC_A2 [mol] | Amount of FCC_A1 [mol] | Amount of GRAPHITE [mol] | Amount of LIQUID [mol] |
| 1000.00000 | 0.99609 | | 0.00391 | |
| 1010.00000 | 0.99618 | | 0.00382 | |
| 1011.17630 | 0.99620 | | 0.00380 | |
| 1011.17630 | 0.99620 | 0.00000 | 0.00380 | |
| 1011.17630 | 0.87367 | 0.12633 | 0.00000 | |
| 1011.17630 | 0.87367 | 0.12633 | | |
| 1020.00000 | 0.86050 | 0.13950 | | |
| 1030.00000 | 0.84335 | 0.15665 | | |
| 1040.00000 | 0.82359 | 0.17641 | | |
| 1050.00000 | 0.80085 | 0.19915 | | |
| 1060.00000 | 0.77399 | 0.22601 | | |
| 1070.00000 | 0.74184 | 0.25816 | | |
| 1080.00000 | 0.70282 | 0.29718 | | |
| 1090.00000 | 0.65470 | 0.34530 | | |
| 1100.00000 | 0.59418 | 0.40582 | | |
| 1110.00000 | 0.51618 | 0.48382 | | |
| 1120.00000 | 0.41250 | 0.58750 | | |
| 1130.00000 | 0.26894 | 0.73106 | | |
| 1140.00000 | 0.05863 | 0.94137 | | |
| 1142.15538 | 0.00000 | 1.00000 | | |
| 1142.15538 | | 1.00000 | | |
| 1150.00000 | | 1.00000 | | |
| 1160.00000 | | 1.00000 | | |
| 1170.00000 | | 1.00000 | | |
| 1180.00000 | | 1.00000 | | |
| 1190.00000 | | 1.00000 | | |
| 1200.00000 | | 1.00000 | | |
| 1210.00000 | | 1.00000 | | |
| 1220.00000 | | 1.00000 | | |

T_03: Fe-C Phase Diagrams

This example shows the stable Fe-C phase diagram (stable meaning that the graphite phase is entered in the calculation). The same diagram is calculated using the Binary Calculator activity and then using a System Definer and Equilibrium Calculator.

In both cases, a Plot Renderer is used to display results. The purpose of the Binary Calculator is to simplify common calculations for binary systems. In the Equilibrium Calculator two axes are defined: *Mass percent C* and *Temperature*. An axis variable must also be an equilibrium condition.

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

- Folder: Thermo-Calc
- File name: *T_03_Fe-C_phase_diagram.tcu*

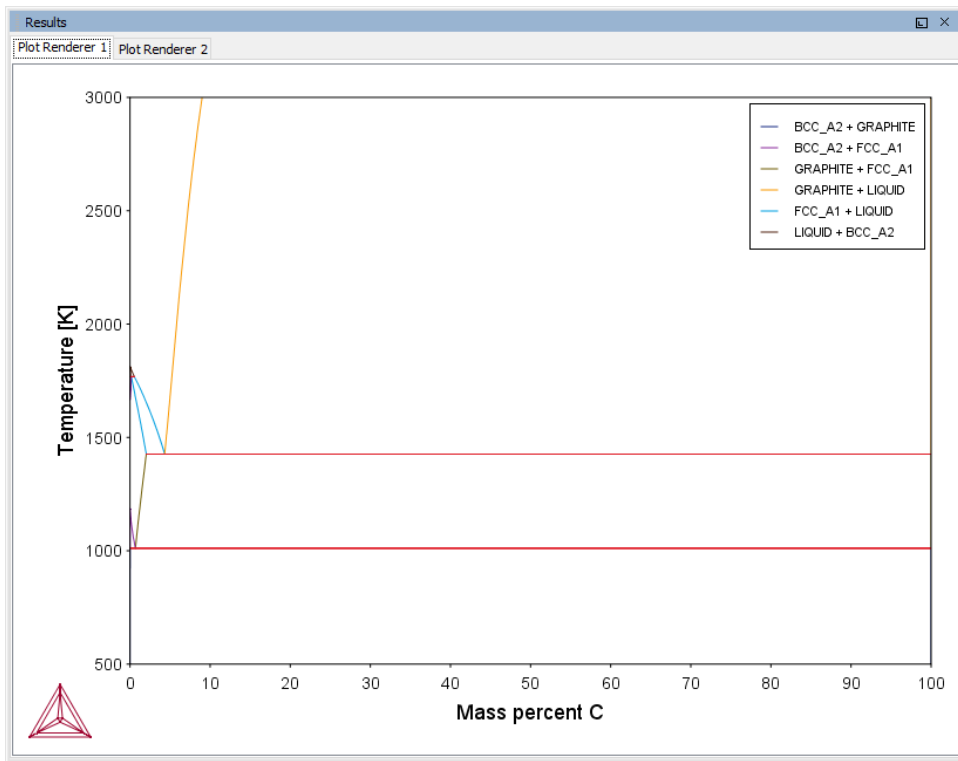


This example is included as a tutorial on our [website](#) and our [YouTube](#) channel.

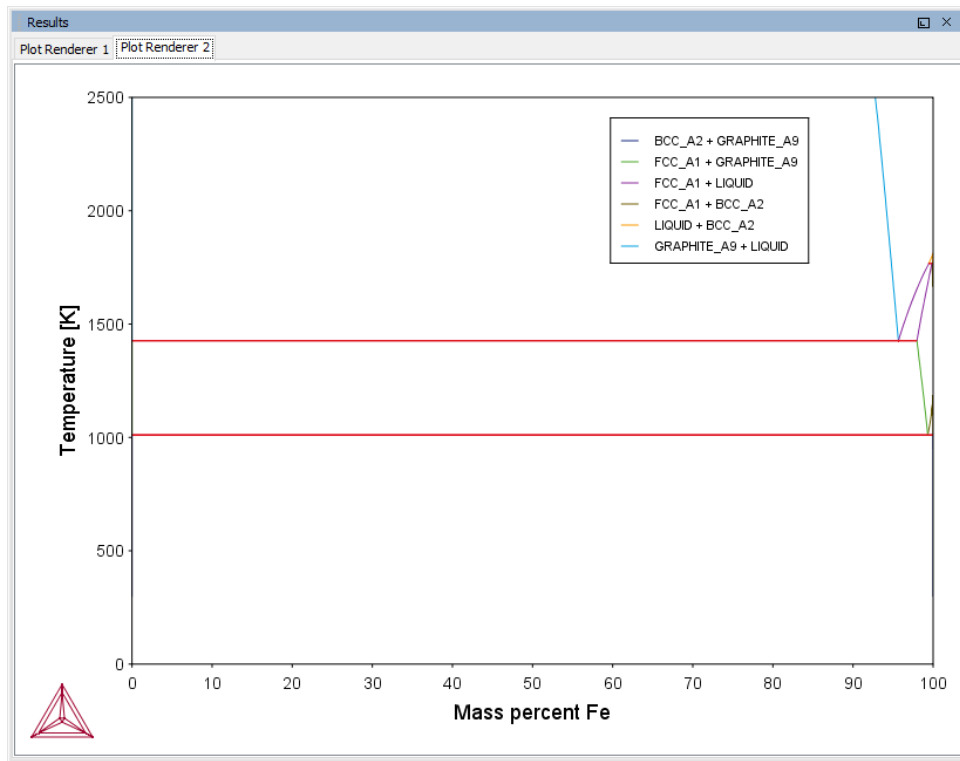
PLOT RESULTS

Equilibrium Calculator Results

This shows the plot result of the System Definer and Equilibrium Calculator system.



Binary Calculator Results



T_04: Fe-Cr-C Ternary Phase Diagram at 1000 K

This example shows a ternary phase diagram in the Fe-Cr-C system at 1000 K. Similar to example "[T_03: Fe-C Phase Diagrams](#)" on page 244, the same diagram is calculated using a Ternary Calculator and then using a System Definer and Equilibrium Calculator. Two Plot Renderer activities are added to create two plots.

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

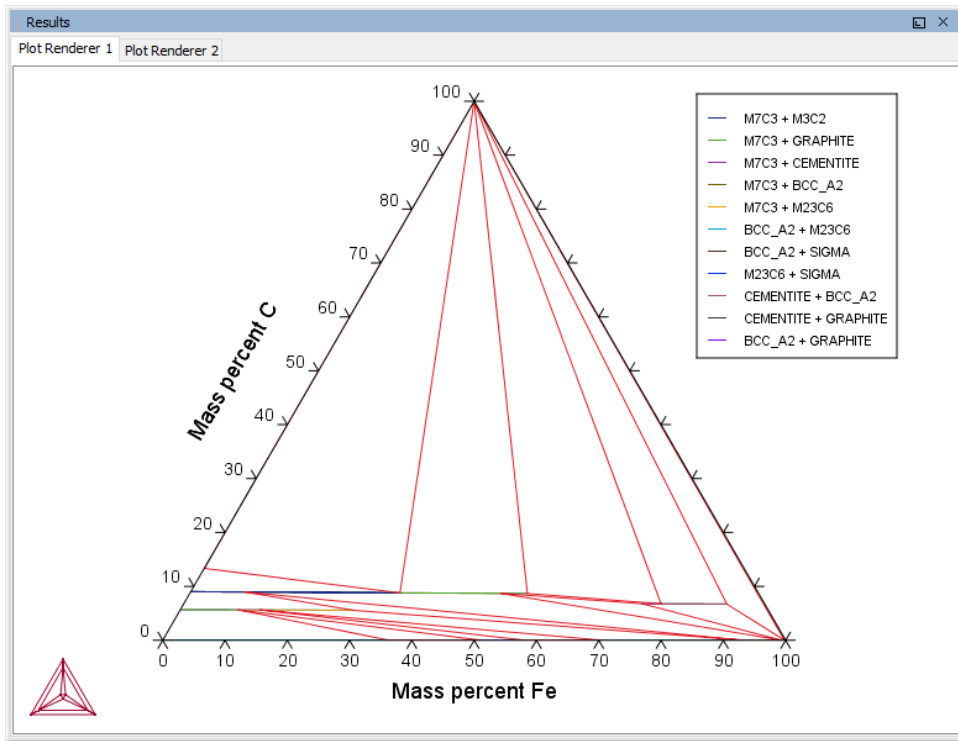
- Folder: Thermo-Calc
- File name: *T_04_Fe-Cr-C_ternary_phase_diagram.tcu*



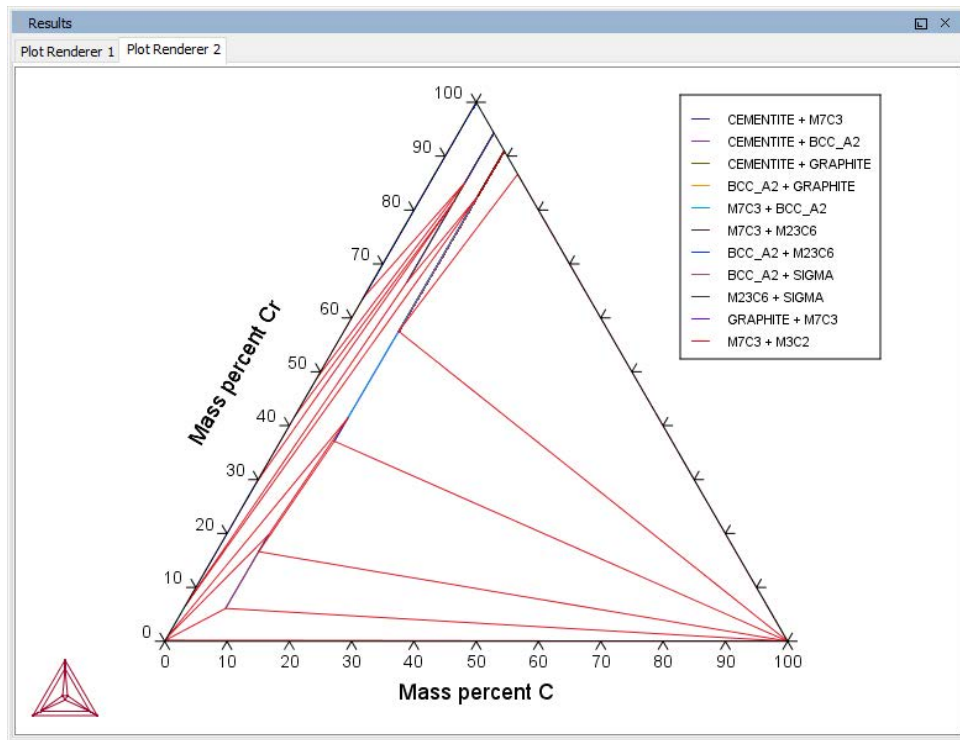
This example is included as a tutorial on our [website](#) and our [YouTube](#) channel.

PLOT RESULTS

Ternary Calculator



Equilibrium Calculator

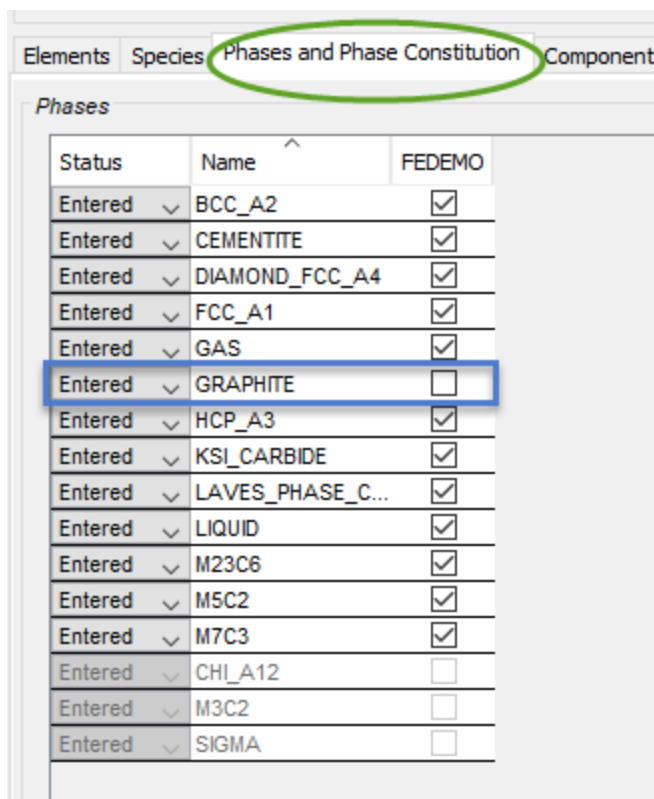


Try practicing with two features on the Plot Renderer Configuration window. To toggle between a triangular and a rectangular diagram, click the **Show Triangular** button then click **Perform** to see what happens. To toggle the X and Y axis variables, click the **Switch Axes** button and then click **Perform**.

T_05: Stable and the Metastable Fe-C Phase Diagrams

This example shows how to overlay results from two calculations in the same plot using the Equilibrium Calculator.

1. The Plot Renderer activity is first created as a successor to Equilibrium Calculator 1.
2. Then right-click the Plot Renderer node and select **Add predecessor** and the results from both equilibrium calculators are in the same plot. In *Equilibrium Calculator 1* the stable phase diagram is calculated and in *Equilibrium Calculator 2* the metastable phase.
3. The metastable diagram is obtained by deselecting the graphite phase on System Definer2 → **Phases and phase constitution** tab.



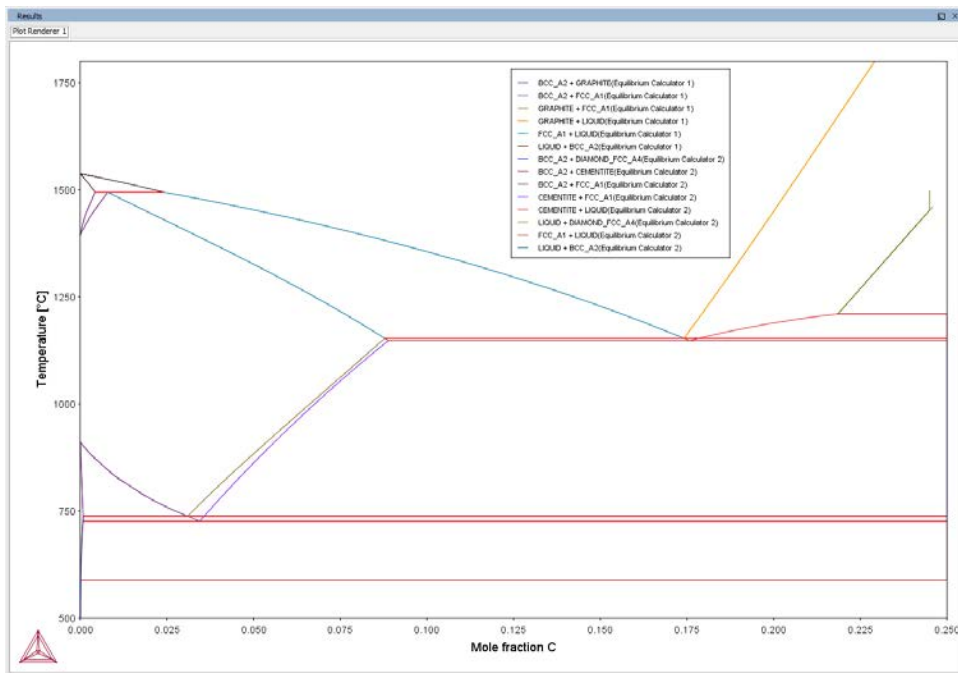
PROJECT FILE AND VIDEO TUTORIAL INFORMATION

- Folder: Thermo-Calc
- File name: T_05_Fe-C_stable_and_metastable_phase_diagram.tcu



You can access video tutorials in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or you can go to the [website](#) or our [YouTube channel](#).

PLOT RESULT



T_06: Serially Coupled Equilibrium Calculators

Sometimes there are multiple solutions for a given set of equilibrium conditions. In other cases the equilibrium calculation does not converge. You can then aid the final calculation by, in effect, telling the software where it should start the search for the equilibrium.

This example shows how to serially couple two Equilibrium Calculator nodes together for more complex equilibrium conditions. For each calculation, the output is to a Table Renderer.

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

- Folder: Thermo-Calc
- File name: *T_06_Serial_equilibrium_calculators.tcu*



You can access video tutorials in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or you can go to the [website](#) or our [YouTube channel](#).

Table Renderer Results

Equilibrium Calculator 1

In the first example, the objective is to calculate the equilibrium at 850° C where the mole fractions of the FCC A1 and BCC A2 phases are 0.5 each for an Fe-Cr-C steel with 10% chromium. In Equilibrium Calculator 1 a simple set of equilibrium conditions (temperature, pressure, system size and composition) are used to find a carbon content where only the FCC A1 and BCC A2 phases are stable. The results from this preliminary calculation are displayed in Table Renderer 1.

| Results | | | | |
|---------------------------------------------------------------------------|----------------------|----------------------|------------------------|------------------|
| Table Renderer 1 Table Renderer 2 Table Renderer 3 Table Renderer 4 | | | | |
| System | | | | |
| Moles | 1.00000 | | | |
| Mass | 55.41634 | [g] | | |
| Temperature | 1123.15000 | [K] | | |
| Total Gibbs Energy | -52361.90905 | [J] | | |
| Enthalpy | 32589.15580 | [J] | | |
| Volume | 7.34406E-6 | [m ³] | | |
| <i>Component</i> | <i>Mole Fraction</i> | <i>Mass Fraction</i> | <i>Activity</i> | <i>Potential</i> |
| C | 0.00046 | 0.00010 | 0.00137 | -61592.91681 |
| Cr | 0.10658 | 0.10000 | 0.00235 | -56531.30746 |
| Fe | 0.89296 | 0.89990 | 0.00387 | -51859.50665 |
| Stable Phases | | | | |
| | <i>Moles</i> | <i>Mass</i> | <i>Volume Fraction</i> | |
| BCC_A2#1 | 0.76777 | 42.55315 | 0.76992 | Composition ▾ |
| Composition | | | | |
| <i>Component</i> | <i>Mole Fraction</i> | <i>Mass Fraction</i> | | |
| Fe | 0.89183 | 0.89864 | | |
| Cr | 0.10801 | 0.10133 | | |
| C | 0.00016 | 0.00003 | | |
| | <i>Moles</i> | <i>Mass</i> | <i>Volume Fraction</i> | |
| FCC_A1#1 | 0.23223 | 12.86320 | 0.23008 | Composition ▾ |
| Composition | | | | |
| <i>Component</i> | <i>Mole Fraction</i> | <i>Mass Fraction</i> | | |
| Fe | 0.89669 | 0.90408 | | |
| Cr | 0.10185 | 0.09560 | | |
| C | 0.00147 | 0.00032 | | |

Equilibrium Calculator 2

In Equilibrium Calculator 2 the carbon content equilibrium condition is replaced by the condition that the numbers of moles of the BCC A2 phase should be 0.5. The final result is displayed in Table Renderer 2. In this case, the final objective is to calculate the solidus temperature of an Fe-Cr-C steel with 10% Cr and 0.01% C.

| Results | | | | |
|---------------------------------------------------------------------------|----------------------|----------------------|------------------------|------------------|
| Table Renderer 1 Table Renderer 2 Table Renderer 3 Table Renderer 4 | | | | |
| System | | | | |
| Moles | 1.00000 | | | |
| Mass | 55.39810 | [g] | | |
| Temperature | 1123.15000 | [K] | | |
| Total Gibbs Energy | -52365.69157 | [J] | | |
| Enthalpy | 32827.91821 | [J] | | |
| Volume | 7.32017E-6 | [m ³] | | |
| <i>Component</i> | <i>Mole Fraction</i> | <i>Mass Fraction</i> | <i>Activity</i> | <i>Potential</i> |
| C | 0.00088 | 0.00019 | 0.00146 | -60967.89084 |
| Cr | 0.10654 | 0.10000 | 0.00238 | -56409.41447 |
| Fe | 0.89258 | 0.89981 | 0.00387 | -51874.52376 |
| Stable Phases | | | | |
| | <i>Moles</i> | <i>Mass</i> | <i>Volume Fraction</i> | |
| BCC_A2#1 | 0.50000 | 27.70824 | 0.50303 | Composition ▾ |
| Composition | | | | |
| <i>Component</i> | <i>Mole Fraction</i> | <i>Mass Fraction</i> | | |
| Fe | 0.89000 | 0.89692 | | |
| Cr | 0.10982 | 0.10304 | | |
| C | 0.00017 | 0.00004 | | |
| | <i>Moles</i> | <i>Mass</i> | <i>Volume Fraction</i> | |
| FCC_A1#1 | 0.50000 | 27.68987 | 0.49697 | Composition ▾ |
| Composition | | | | |
| <i>Component</i> | <i>Mole Fraction</i> | <i>Mass Fraction</i> | | |
| Fe | 0.89515 | 0.90270 | | |
| Cr | 0.10326 | 0.09695 | | |
| C | 0.00159 | 0.00034 | | |

Equilibrium Calculator 3

In Equilibrium Calculator 3 the state at 2000 K is calculated and the result is displayed in Table Renderer 3.

| Results | | | | |
|---------------------------------------------------------------------------|----------------------|----------------------|------------------------|------------------|
| Table Renderer 1 Table Renderer 2 Table Renderer 3 Table Renderer 4 | | | | |
| System | | | | |
| Moles | 1.00000 | | | |
| Mass | 55.41634 | [g] | | |
| Temperature | 1123.15000 | [K] | | |
| Total Gibbs Energy | -52361.90905 | [J] | | |
| Enthalpy | 32589.15580 | [J] | | |
| Volume | 7.34406E-6 | [m ³] | | |
| <i>Component</i> | <i>Mole Fraction</i> | <i>Mass Fraction</i> | <i>Activity</i> | <i>Potential</i> |
| C | 0.00046 | 0.00010 | 0.00137 | -61592.91681 |
| Cr | 0.10658 | 0.10000 | 0.00235 | -56531.30746 |
| Fe | 0.89296 | 0.89990 | 0.00387 | -51859.50665 |
| Stable Phases | | | | |
| | <i>Moles</i> | <i>Mass</i> | <i>Volume Fraction</i> | |
| BCC_A2#1 | 0.76777 | 42.55315 | 0.76992 | Composition ▾ |
| Composition | | | | |
| <i>Component</i> | <i>Mole Fraction</i> | <i>Mass Fraction</i> | | |
| Fe | 0.89183 | 0.89864 | | |
| Cr | 0.10801 | 0.10133 | | |
| C | 0.00016 | 0.00003 | | |
| | <i>Moles</i> | <i>Mass</i> | <i>Volume Fraction</i> | |
| FCC_A1#1 | 0.23223 | 12.86320 | 0.23008 | Composition ▾ |
| Composition | | | | |
| <i>Component</i> | <i>Mole Fraction</i> | <i>Mass Fraction</i> | | |
| Fe | 0.89669 | 0.90408 | | |
| Cr | 0.10185 | 0.09560 | | |
| C | 0.00147 | 0.00032 | | |

Equilibrium Calculator 4

In Equilibrium Calculator 4 the temperature equilibrium condition is replaced by the condition *Fix phase / liquid / 0.0*, meaning that liquid should be stable in an amount of zero moles, i.e. the solidus temperature. The final result is displayed in Table Renderer 4.

| Results | | | | |
|---------------------------------------------------------------------------|----------------------|----------------------|------------------------|------------------|
| Table Renderer 1 Table Renderer 2 Table Renderer 3 Table Renderer 4 | | | | |
| System | | | | |
| Moles | 1.00000 | | | |
| Mass | 55.41634 | [g] | | |
| Temperature | 1791.51760 | [K] | | |
| Total Gibbs Energy | -1.09463E5 | [J] | | |
| Enthalpy | 59070.77313 | [J] | | |
| Volume | 7.63568E-6 | [m3] | | |
| <i>Component</i> | <i>Mole Fraction</i> | <i>Mass Fraction</i> | <i>Activity</i> | <i>Potential</i> |
| C | 0.00046 | 0.00010 | 0.00012 | -1.34945E5 |
| Cr | 0.10658 | 0.10000 | 0.00030 | -1.20950E5 |
| Fe | 0.89296 | 0.89990 | 0.00071 | -1.08079E5 |
| Stable Phases | | | | |
| | <i>Moles</i> | <i>Mass</i> | <i>Volume Fraction</i> | |
| BCC_A2#1 | 1.00000 | 55.41634 | 1.00000 | Composition ▾ |
| Composition | | | | |
| <i>Component</i> | <i>Mole Fraction</i> | <i>Mass Fraction</i> | | |
| Fe | 0.89296 | 0.89990 | | |
| Cr | 0.10658 | 0.10000 | | |
| C | 0.00046 | 0.00010 | | |
| Fixed Phases | | | | |
| | <i>Moles</i> | <i>Mass</i> | <i>Volume Fraction</i> | |
| LIQUID#1 | 0.00000 | 0.00000 | 0.00000 | Composition ▾ |
| Composition | | | | |
| <i>Component</i> | <i>Mole Fraction</i> | <i>Mass Fraction</i> | | |
| Fe | 0.88607 | 0.89447 | | |
| Cr | 0.11178 | 0.10506 | | |
| C | 0.00216 | 0.00047 | | |

T_07: User-Defined Functions

This example shows how to implement user-defined functions.

A series of equilibria for an Fe-Cr-C alloy are calculated by varying temperature between 500 and 3000 K. In the configuration window of the Equilibrium Calculator under the **Functions** tab, two identically meaning functions are defined, *fraction solid* and *f solid*, the values of which are plotted against temperature in two Plot Renderer activities. Functions can be entered in terms of *QuantitiesQ1*, *Q2*, *Q3* and so forth, or by using the Thermo-Calc syntax.

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

- Folder: Thermo-Calc
- File name: *T_07_User_defined_functions.tcu*



You can access video tutorials in a variety of ways. When in Thermo-Calc, from the menu select **Help → Video Tutorials**, or you can go to the [website](#) or our [YouTube channel](#).

PLOT RESULT

This plot example shows the result of the fraction solid function.

Equilibrium Calculator 1

Legend option: Legend style:

X-axis

Axis variable:

Axis type:

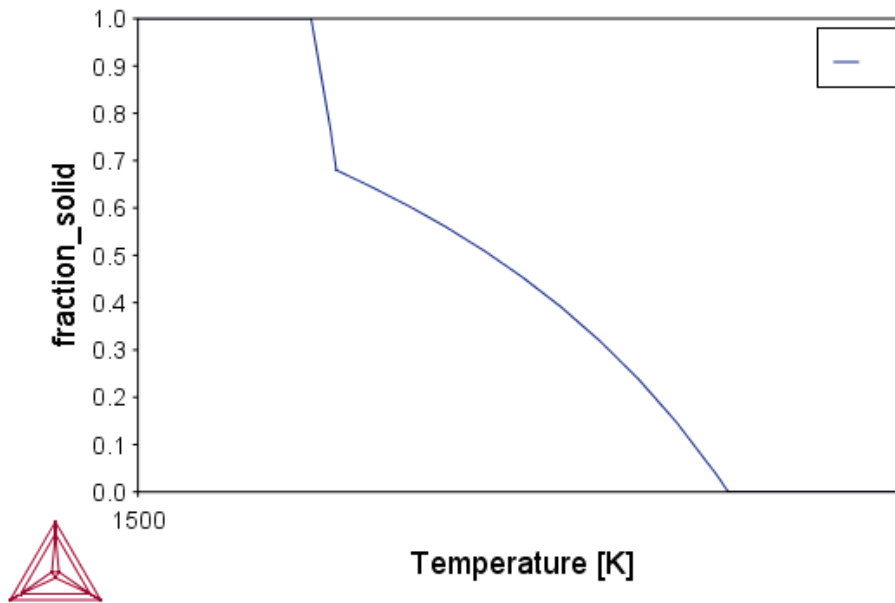
Limits: to step ☐ Automatic scaling

Y-axis

Axis variable:

Axis type:

Limits: to step ☐ Automatic scaling



T_08: Scheil and Equilibrium Solidification

This example shows a comparison for an Al-Si alloy solidified under full local equilibrium and under the Scheil assumptions, i.e. zero diffusion in the solidified material and infinitely fast diffusion in the liquid. The example uses the Scheil Calculator and adds a Plot and Table Renderer.

▶ ["T_10: Scheil Solidification with Back Diffusion" on page 263](#)

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

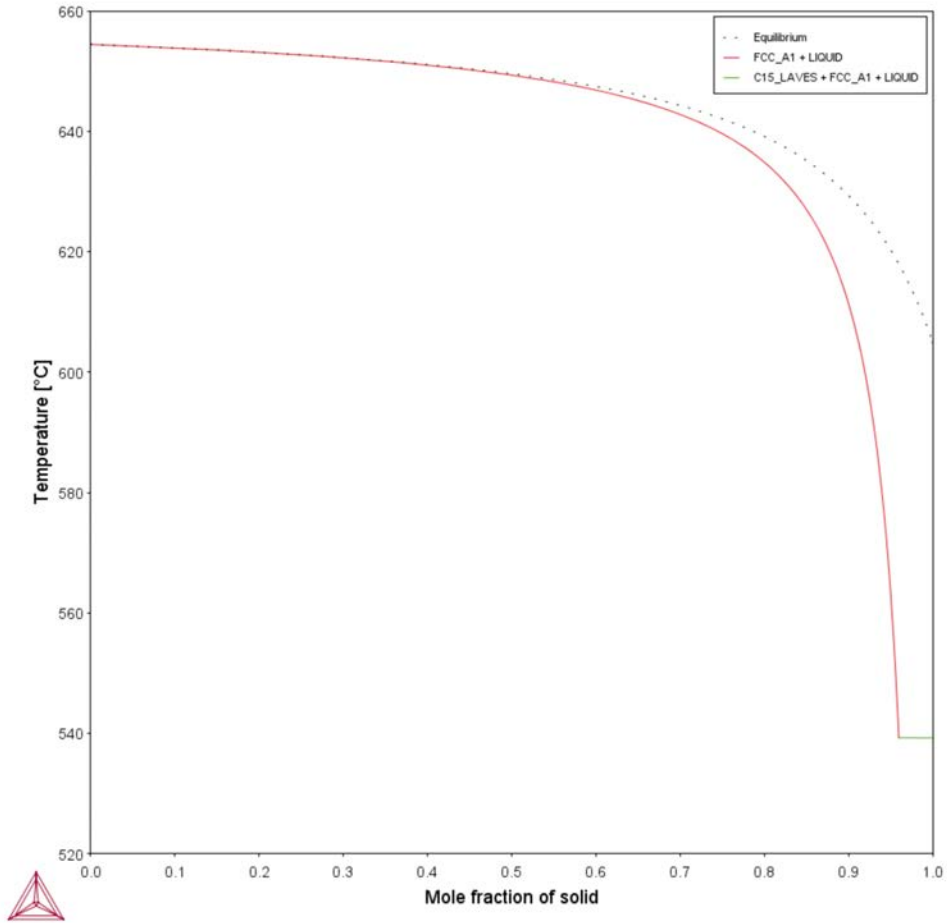
- Folder: Thermo-Calc
- File name: *T_08_Scheil_and_equilibrium_solidification.tcu*.



For video tutorial examples using Scheil, see our [website](#) and [YouTube channel](#).

TABLE AND PLOT RESULTS

The plot compares the mole fraction of a solid vs temperature. The table provides the data, which you can also export.



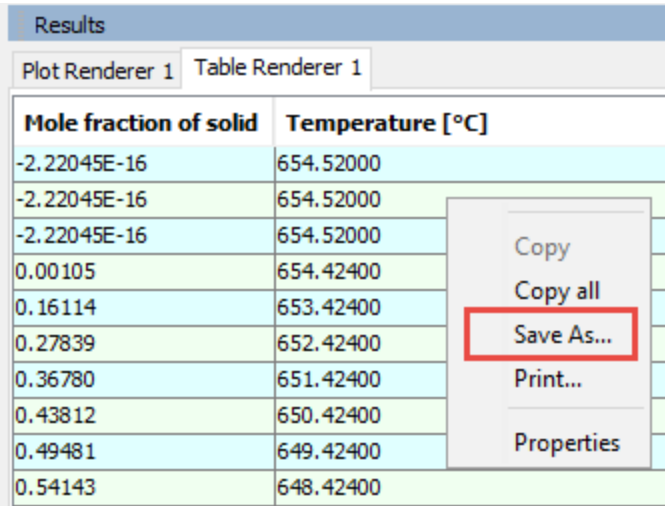
| Results | |
|------------------------|------------------|
| Plot Renderer 1 | Table Renderer 1 |
| Mole fraction of solid | Temperature [°C] |
| -2.22045E-16 | 654.52000 |
| -2.22045E-16 | 654.52000 |
| -2.22045E-16 | 654.52000 |
| 0.00105 | 654.42400 |
| 0.16114 | 653.42400 |
| 0.27839 | 652.42400 |
| 0.36780 | 651.42400 |
| 0.43812 | 650.42400 |
| 0.49481 | 649.42400 |
| 0.54143 | 648.42400 |

To SAVE THE TABLE

There are two ways to save the table.

Method 1

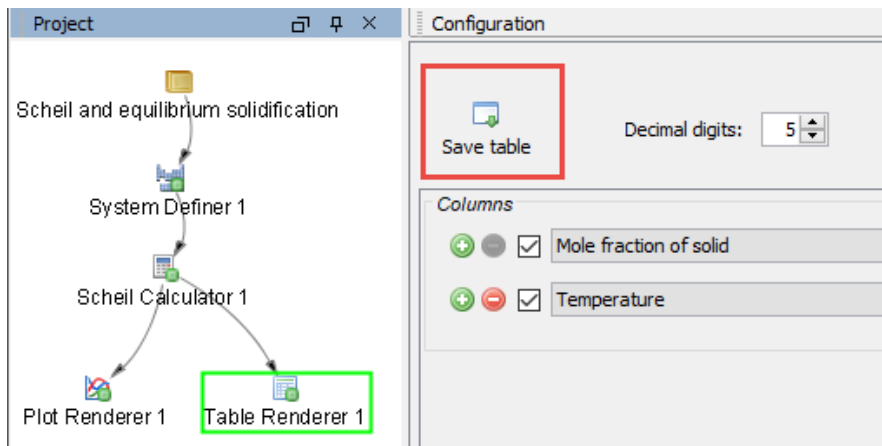
In the **Results** window, right click the table and select **Save As...**



| Mole fraction of solid | Temperature [°C] |
|------------------------|------------------|
| -2.22045E-16 | 654.52000 |
| -2.22045E-16 | 654.52000 |
| -2.22045E-16 | 654.52000 |
| 0.00105 | 654.42400 |
| 0.16114 | 653.42400 |
| 0.27839 | 652.42400 |
| 0.36780 | 651.42400 |
| 0.43812 | 650.42400 |
| 0.49481 | 649.42400 |
| 0.54143 | 648.42400 |

Method 2

1. In the **Project** window, click the **Table Renderer**.
2. In the **Configuration** window, click **Save table**.



T_09: Carbide Driving Force Heat Map

This is an example of using *Grid* calculations to plot the driving force for a carbide as a function of two composition variables. With the *Grid* calculation type, a 2D grid is generated from the two calculation axes. After the calculation is done, an equilibrium is calculated in each grid point. A "[Plot Renderer](#)" on [page 179](#) connected to a grid calculation plots the z-axis property for each equilibrium as a function of the two calculation axes. The final plot can be either a heat map or a contour plot.

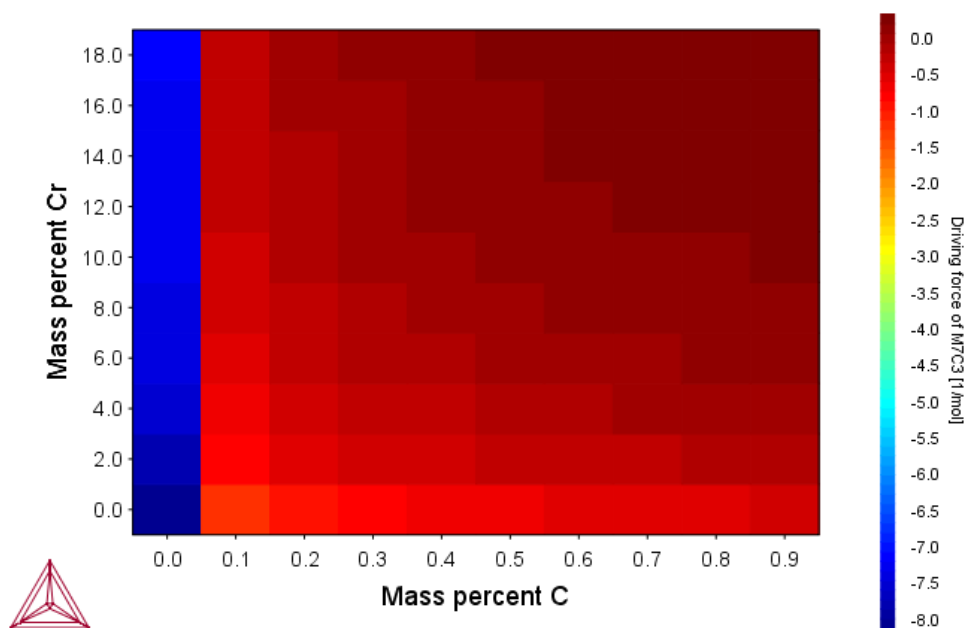
PROJECT FILE AND VIDEO TUTORIAL INFORMATION

- Folder: Thermo-Calc
- File name: *T_09_Heat_map_of_carbide_driving_force.tcu*



You can access video tutorials in a variety of ways. When in Thermo-Calc, from the menu select **Help** → **Video Tutorials**, or you can go to the [website](#) or our [YouTube channel](#).

PLOT RESULT



T_10: Scheil Solidification with Back Diffusion

▶ See "[Scheil Calculator](#)" on page 66 for an overview of the different Scheil simulation models available.



The Scheil with back diffusion feature is only available for systems with diffusion data, i.e. it requires the use of a mobility database.

This is an example of a Scheil solidification simulation of a Al-2.1Cu-1Si alloy including back diffusion in the primary phase.

The example uses two of the Scheil Calculator activity nodes with different cooling rates, 10 K/s and 0.005 K/s. The lower cooling rate produces a solidification curve that is closer to the equilibrium curve as shown in the plot result. Both a thermodynamic ALDEMO (aluminum demo) and mobility MALDEMO (Al-alloys mobility) database are used for this calculation.

▶ "[T_08: Scheil and Equilibrium Solidification](#)" on page 258

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

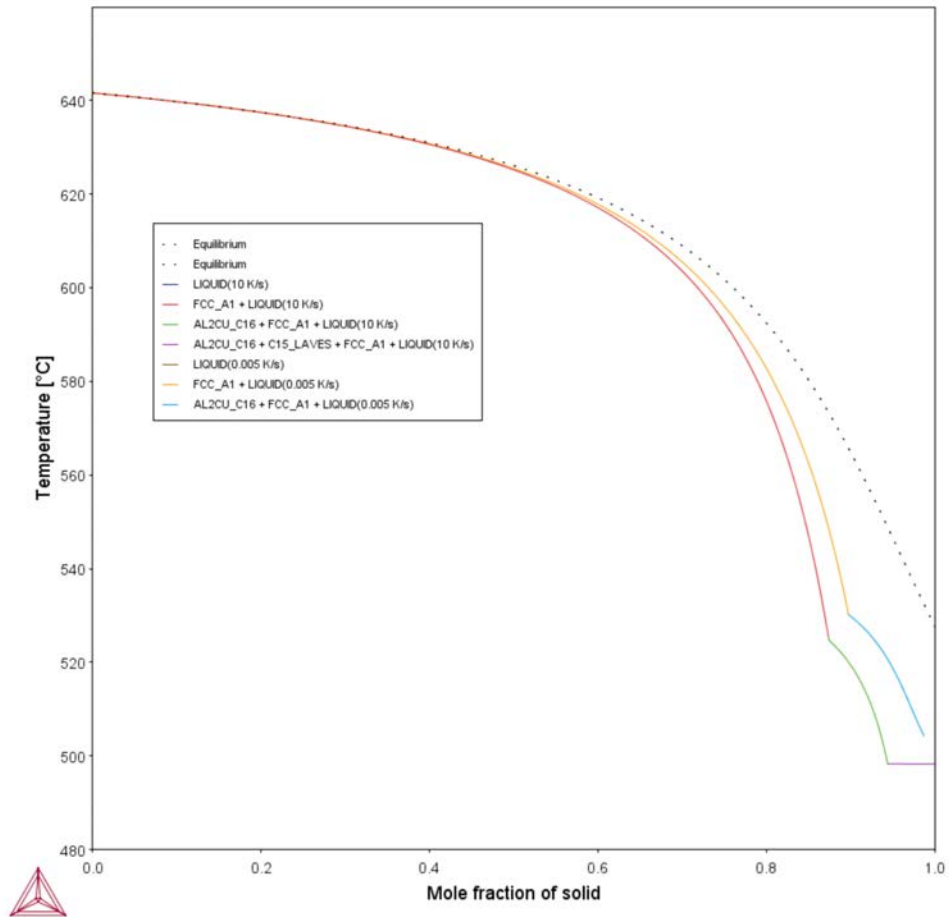
- Folder: Thermo-Calc
- File name: *T_10_Scheil_with_back_diffusion.tcu*.



For video tutorial examples using Scheil, see our [website](#) and [YouTube channel](#).

PLOT RESULT

Scheil Solidification Plot



Thermo-Calc Property Model Examples Collection



The **General models** are available to all users. To run calculations with the **Steel models** (martensite and pearlite) requires a valid maintenance license plus licenses for both the TCFE9 and MOBFE4 databases.

These examples use the **Property Model Calculator**, an activity available with Thermo-Calc.



["About the Examples " on page 23](#)

PM_G_01: Phase Transition

The example uses the Property Model Calculator to predict the transition temperature to the unwanted brittle Sigma phase. The example shows how the temperature is influenced by changes to a steel alloy's composition using the *uncertainty* calculation type and how to create either a *histogram* or *probability* plot.



["Phase Transition Model" on page 83](#) in the *Thermo-Calc User Guide*.

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

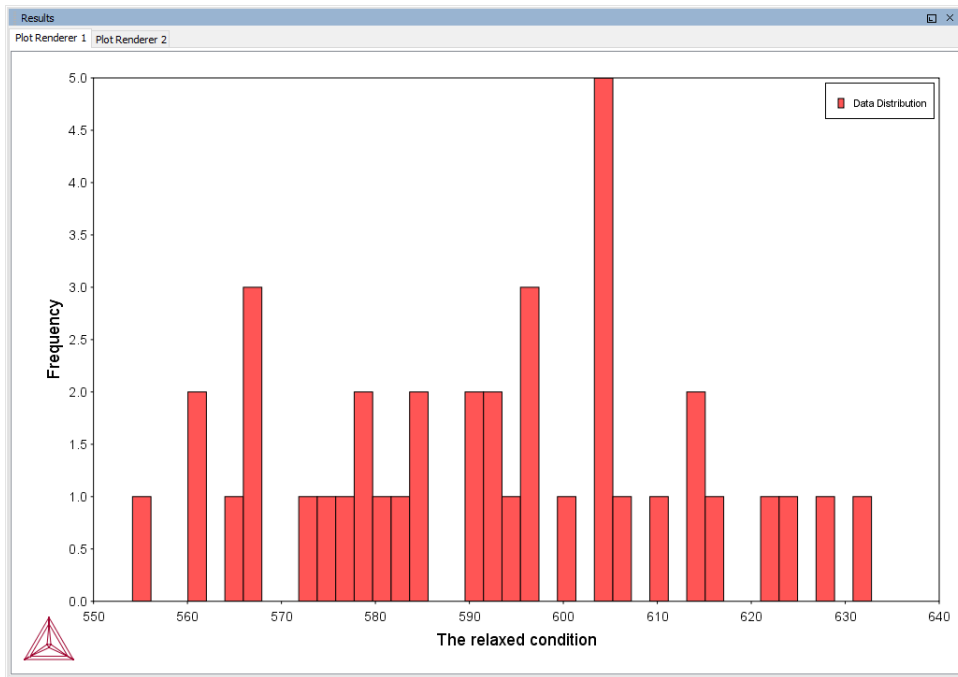
- Folder: Property models>General
- File name: *PM_G_01_Phase_Transition.tcu*



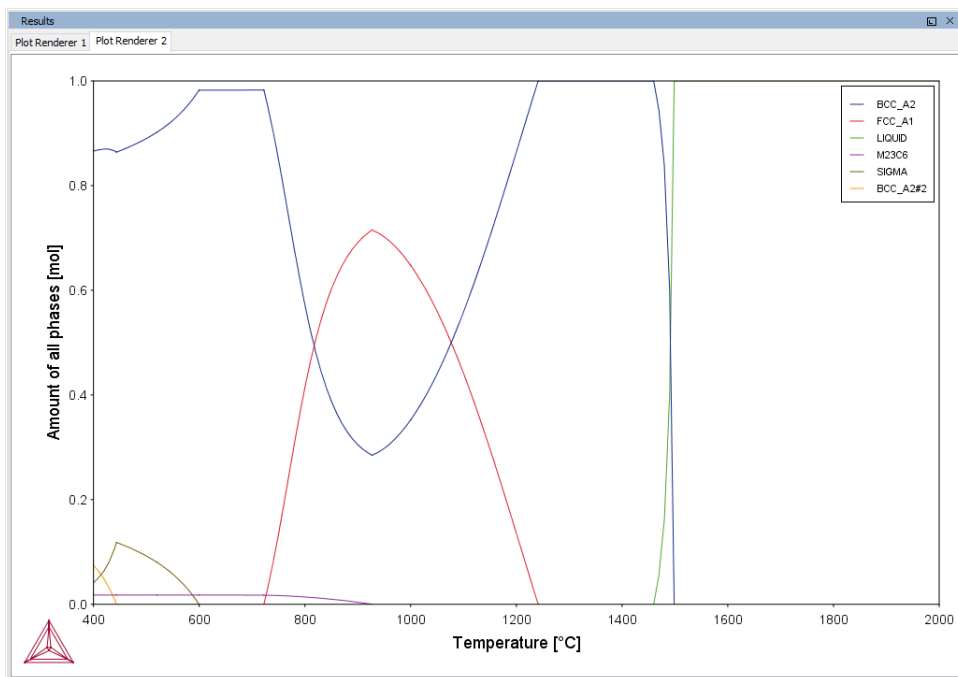
This example is included as a tutorial on our [website](#) and our [YouTube](#) channel.

PLOT RESULTS

Histogram plot



Probability plot





Experienced users can also create custom property models for use with the Property Model Calculator.

- ▶ Search for Property Model Calculator and Development Framework in the help.

PM_G_02: Coarsening and Interfacial Energy

The example uses the Property Model Calculator and both thermodynamic (FEDEMO) and kinetic (MFEDEMO) demonstration steel databases. Using a *Grid* calculation type it produces these plots: a *heat map*, a *contour plot* and a *cross plot with contour* (where both the interfacial energy and coarsening rate is shown). It also creates a diagram to show the phase fractions vs time and a 3D plot comparing the coarsening rate coefficient.

- ▶ ["Coarsening Model" on page 78](#) and ["Interfacial Energy Model" on page 81](#)

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

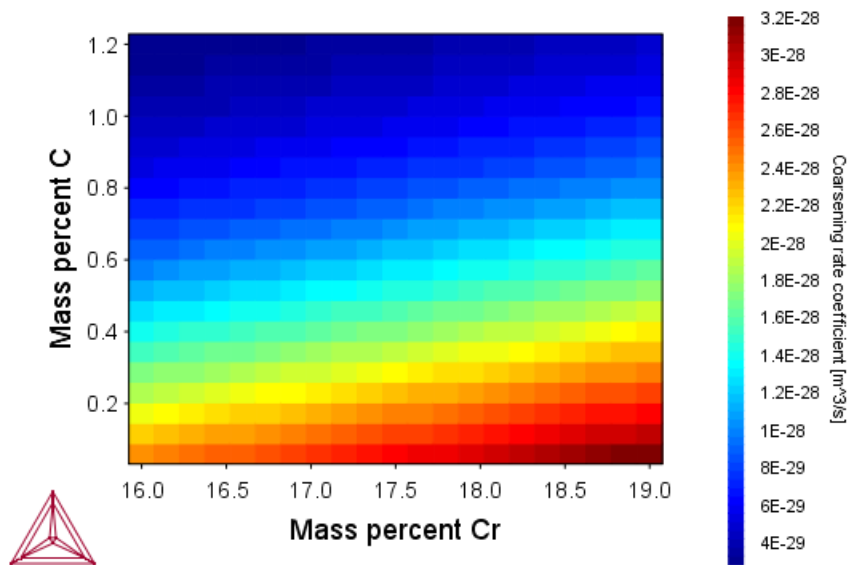
- Folder: Property models>General
- File name: *PM_G_02_Coarsening_and_Interfacial_energy.tcu*



This example is included as a tutorial on our [website](#) and our [YouTube](#) channel.

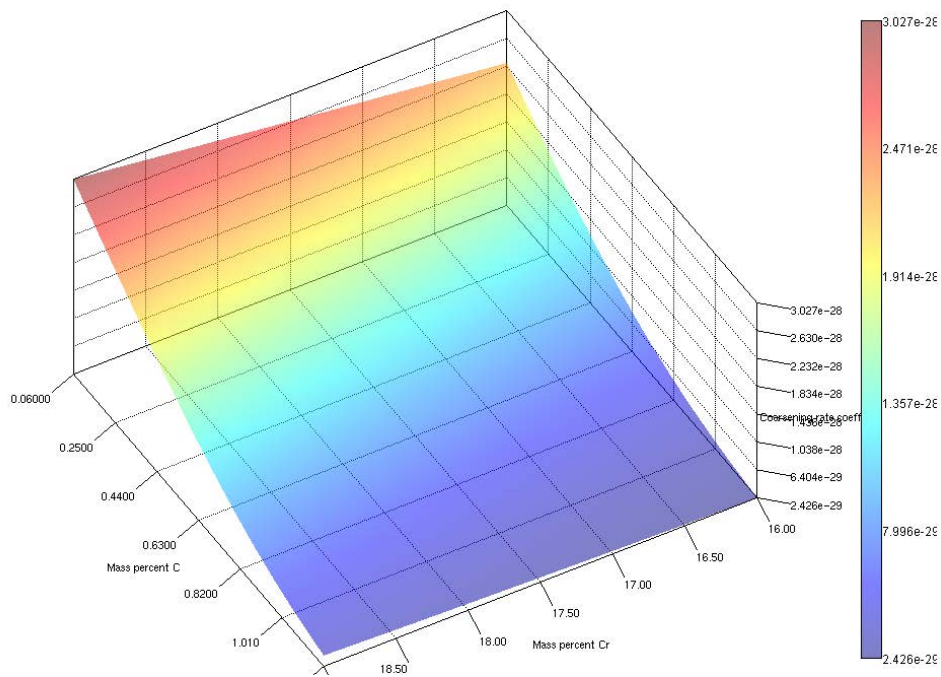
Plot Results

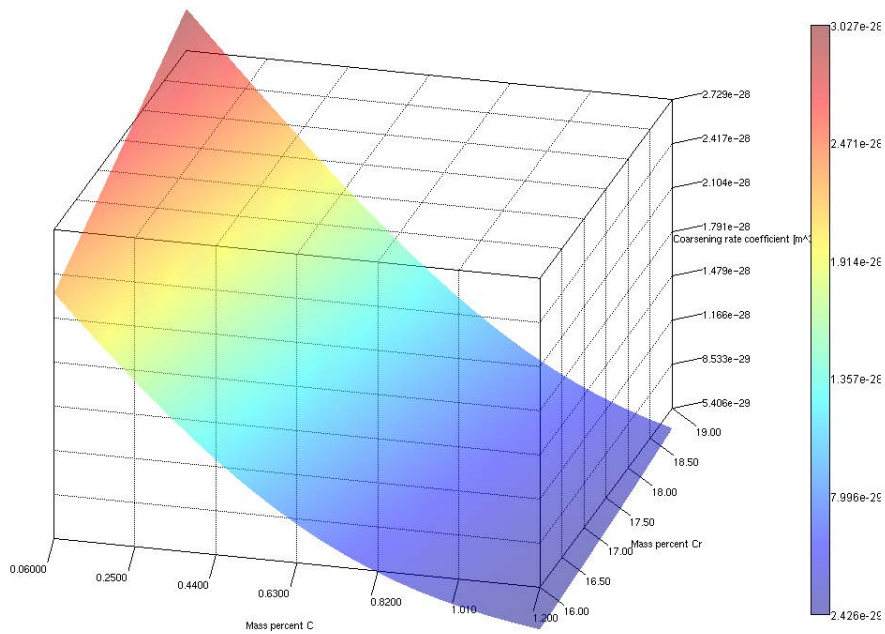
Coarsening rate coefficient (heat map)



Coarsening rate coefficient (3D plot)

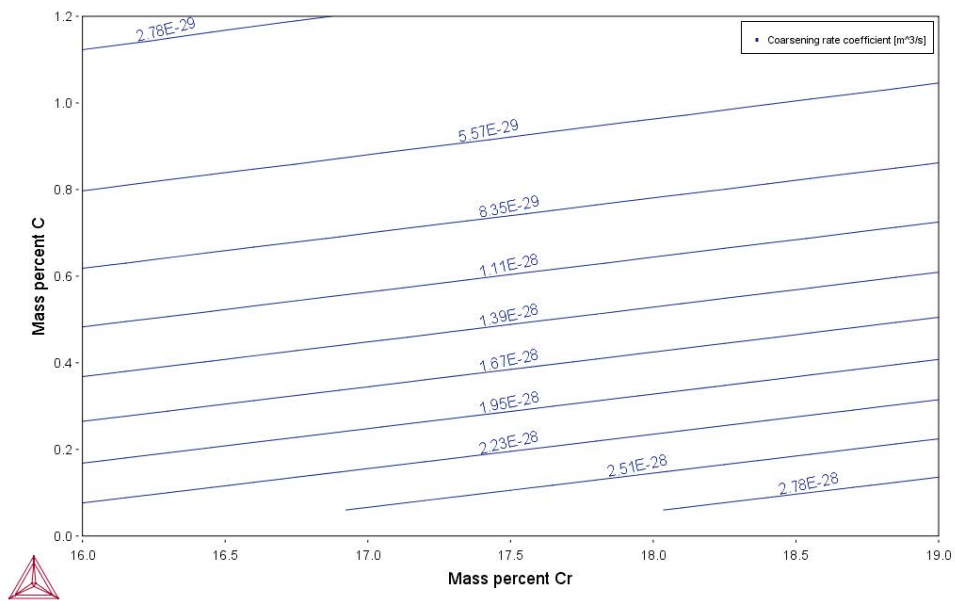
Two different rotation angles. When viewing in Thermo-Calc you can rotate the plot.



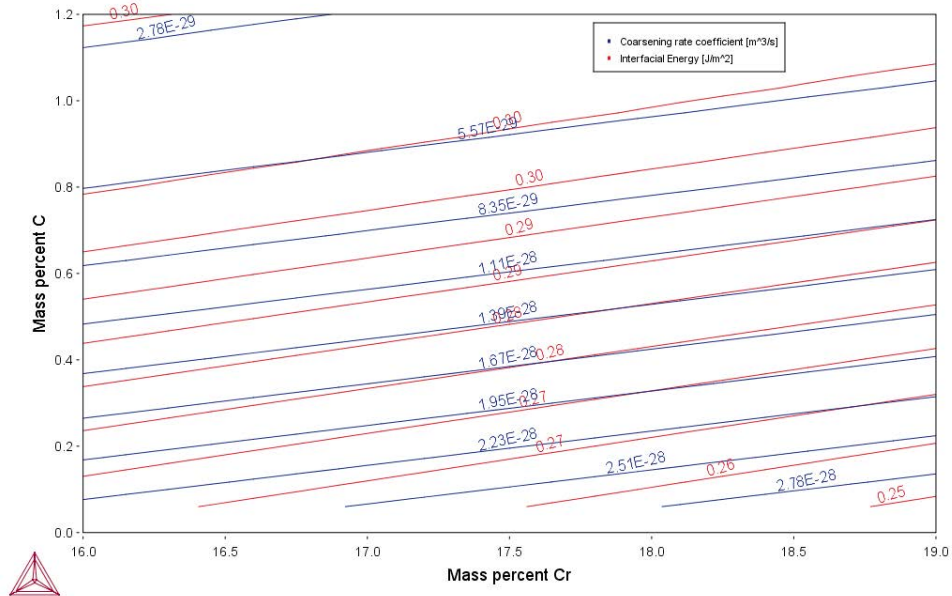


Coarsening rate coefficient (contour plot)

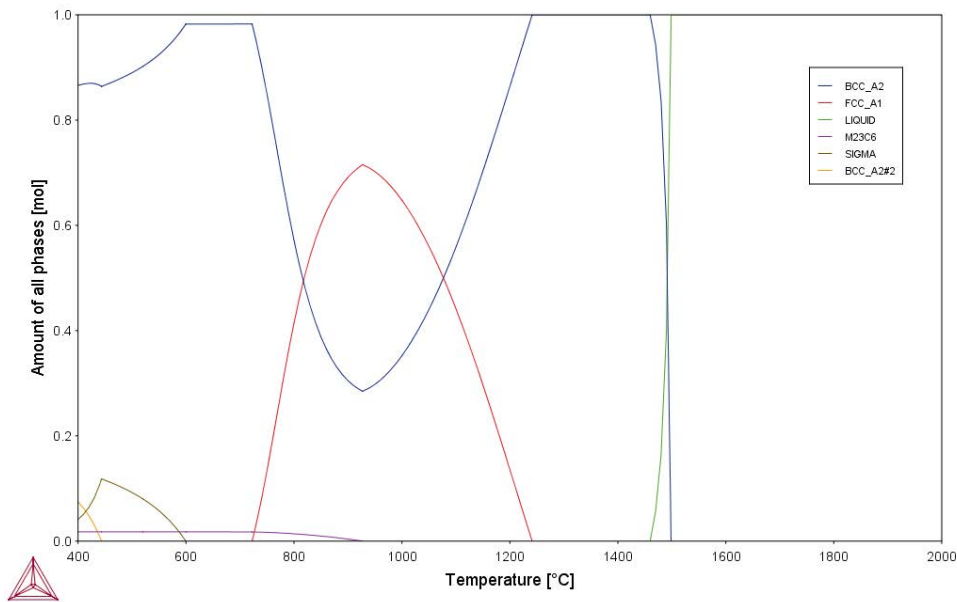
Coarsening rate coefficient



Coarsening rate coefficient and Interfacial energy (overlaid plots)



Phase fractions vs T (One axis)



Experienced users can also create custom property models for use with the Property Model Calculator.

-
- ▶ Search for Property Model Calculator and Development Framework in the help.

PM_G_03: Driving Force and Interfacial Energy

The example uses the Property Model Calculator and a thermodynamic demonstration steel database (FEDEMO). Using a *grid* calculation type it produces a *contour* plot comparing the driving force and interfacial energy.

- ▶ ["Driving Force Model" on page 80](#) and ["Interfacial Energy Model" on page 81](#) in the *Thermo-Calc User Guide*.

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

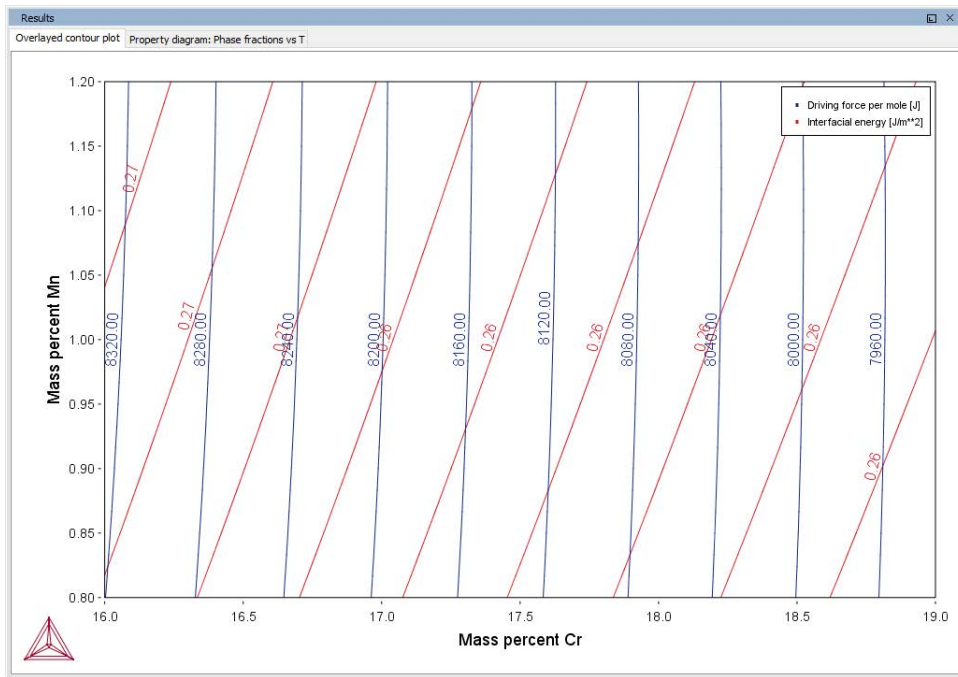
- Folder: Property models>General
- File name: *PM_G_03_Driving_force_and_Interfacial_energy.tcu*



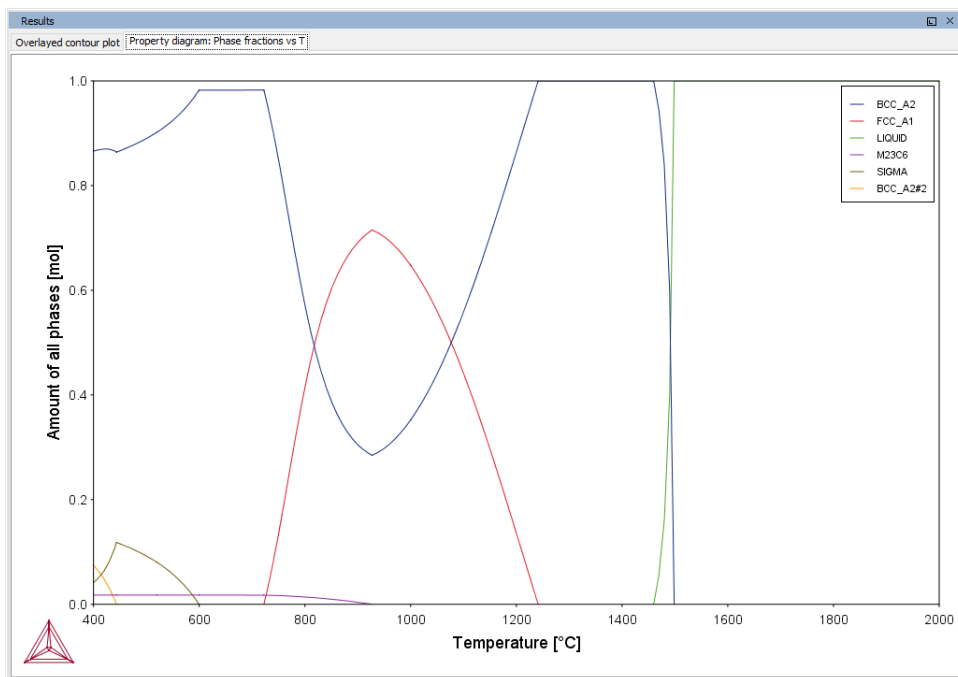
This example is included as a tutorial on our [website](#) and our [YouTube](#) channel.

PLOT RESULT

A contour plot



Phase Fraction





Experienced users can also create custom property models for use with the Property Model Calculator.

- ▶ Search for Property Model Calculator and Development Framework in the help.

PM_G_04_Yield_Strength

- ▶ ["Yield Strength Model" on page 84](#) and ["About the Yield Strength Model" on page 89](#) in the *Thermo-Calc User Guide*.

The example uses the **Property Model Calculator** and the **Yield strength** property model with a thermodynamic demonstration aluminum database (ALDEMO).

This example compares the **Simplified** and **Seidman** models yield strength versus precipitate radius to experimental data for an Al-0.3wt%Sc alloy homogenized at 648 °C for 24 hours and subsequently aged at 350 °C. Although the experimental set up is designed to eliminate grain boundary and solid solution strengthening, these are also included by optimizing the model parameters.

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

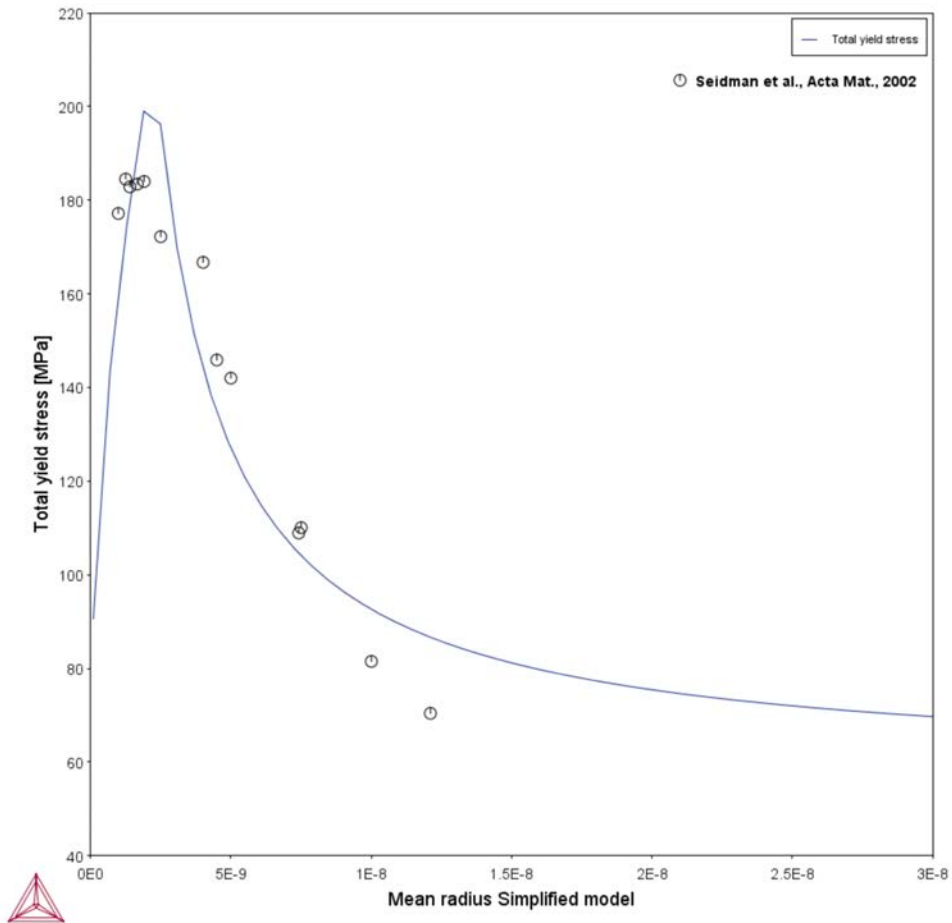
- Folder: Property models>General
- File name: *PM_G_04_Yield_Strength.tcu*



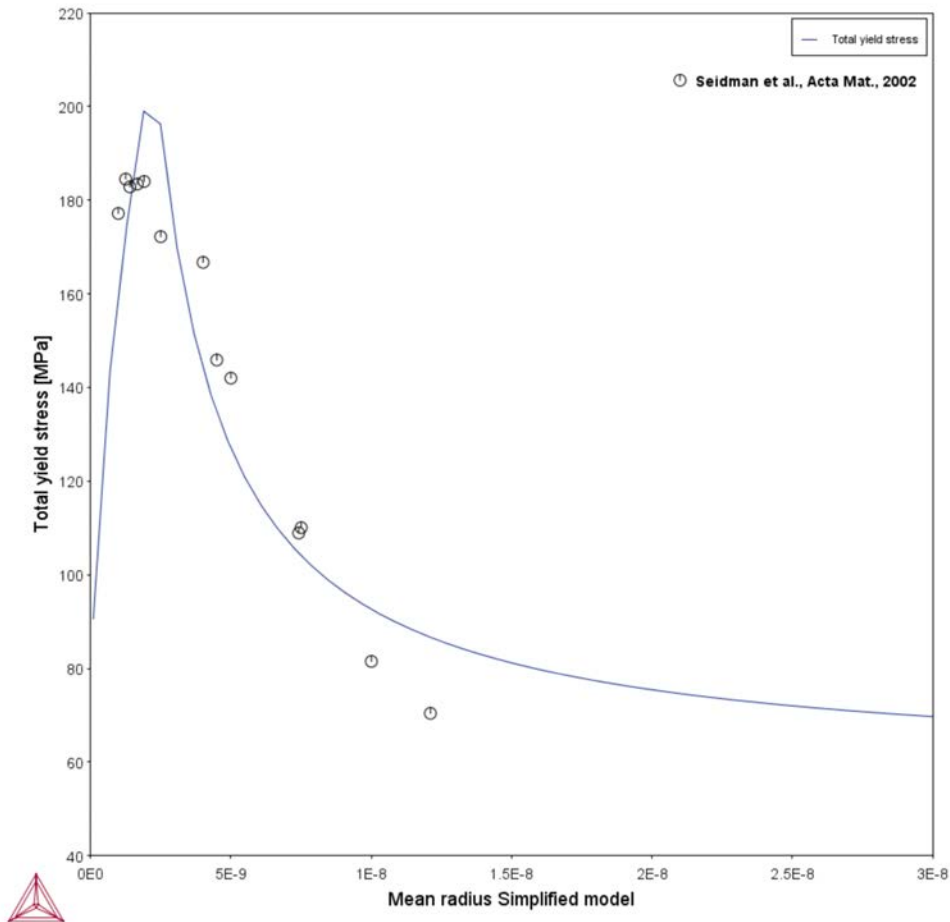
Also see our [website](#) and [YouTube channel](#) for tutorial videos related to the Property Model Calculator.

PLOT RESULT

Strength vs Radius - Simplified



Strength vs Radius - Seidman



Experienced users can also create custom property models for use with the Property Model Calculator.

- ▶ Search for Property Model Calculator and Development Framework in the help.

PM_G_05_Yield_Strength_NiAlCr

- ▶ ["Yield Strength Model" on page 84](#) and ["About the Yield Strength Model" on page 89](#) in the *Thermo-Calc Graphical Mode User Guide*.

The example uses the **Property Model Calculator** and the **Yield strength** property model with a thermodynamic demonstration nickel database (NIDEMO).

The Reppich model is developed for calculation of precipitation strengthening in Ni-based super alloys consisting mainly of gamma prime precipitates in a gamma matrix. The example shows a calculation of the precipitation strengthening vs precipitate radius in a Ni-10at%Al-10at%Cr alloy.

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

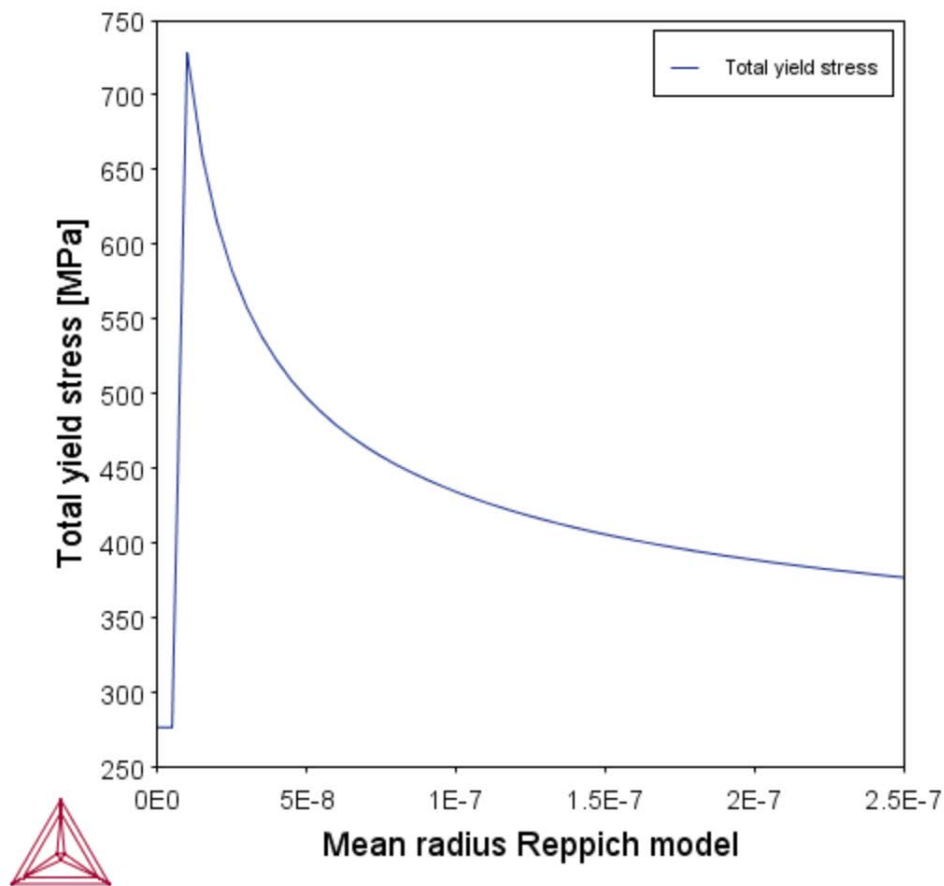
- Folder: Property models>General
- File name: *PM_G_05_Yield_Strength_NiAlCr.tcu*



Also see our [website](#) and [YouTube channel](#) for tutorial videos related to the Property Model Calculator.

PLOT RESULT

Mean Radius Reppich Model



Reppich model plotted with results and experimental data for PE16, all data is normalized with the square root of the volume fraction of precipitate.



Experienced users can also create custom property models for use with the Property Model Calculator.

- ▶ Search for Property Model Calculator and Development Framework in the help.

PM_G_06_Yield_Strength_HEA

- ▶ ["Yield Strength Model" on page 84](#) and ["About the Yield Strength Model" on page 89](#) in the *Thermo-Calc Graphical Mode User Guide*.



This example requires the use of the TCS High Entropy Alloy (TCHEA) database. A license is required to run the example.

The example uses the **Property Model Calculator** and the **Yield strength** property model with a thermodynamic high entropy alloy database (TCHEA). This is an example of solid solution strengthening, which is the contribution to total strength due to the elastic strains in the crystal lattice caused by alloying elements of a lattice parameter differing from the main constituent. The example shows the solid solution strengthening over the full solubility range for the Mo-Ta system as compared to experimental data.

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

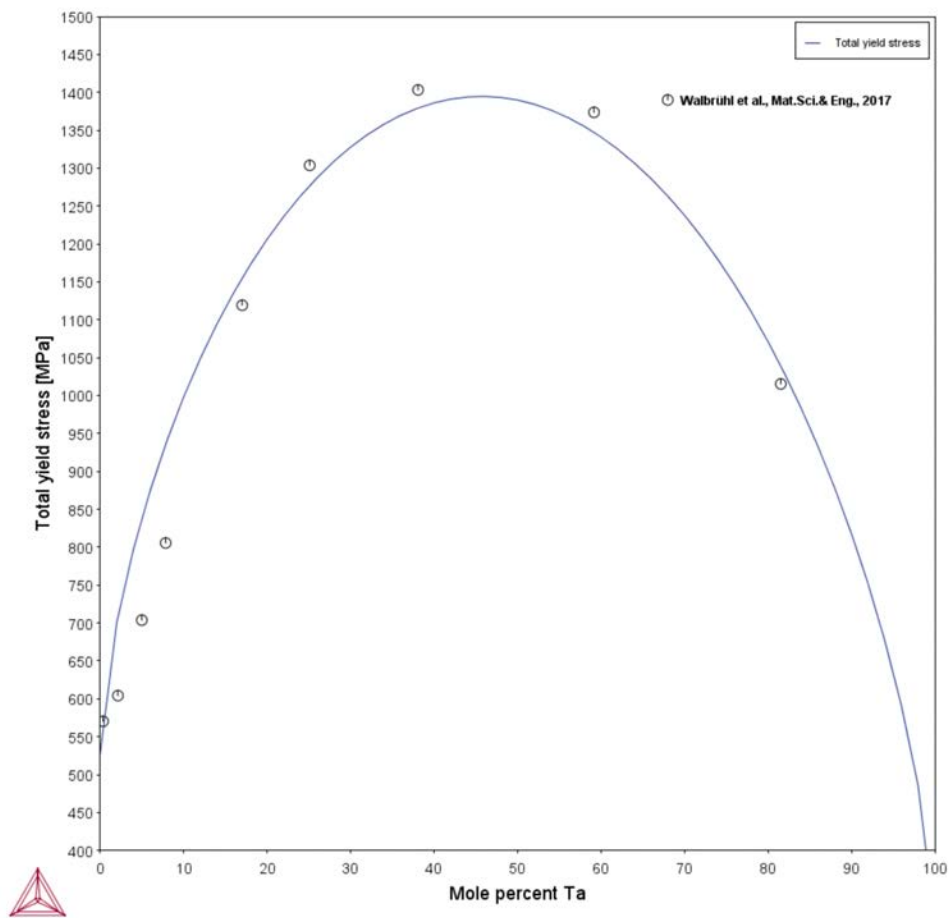
- Folder: Property models>General
- File name: *PM_G_06_Yield_Strength_HEA.tcu*



Also see our [website](#) and [YouTube channel](#) for tutorial videos related to the Property Model Calculator.

PLOT RESULT

Strength vs at% Ta





Experienced users can also create custom property models for use with the Property Model Calculator.



Search for Property Model Calculator and Development Framework in the help.

PM_Fe_01: Fe-Cr-C Martensite with Intercritical Annealing



To run calculations with the **Steel models** (martensite and pearlite) requires a valid maintenance license plus licenses for both the TCFE9 and MOBFE4 databases.

The example uses the Property Model Calculator with the **Martensite Fractions** and **Martensite Temperatures** models.

The example shows how to calculate martensite fractions and martensite temperatures (martensite start, M_s , and 90% transformation temperature M_{90}). The alloy is first intercritically annealed and then quenched. Austenite composition is determined by an equilibrium calculation at the annealing temperature. Martensite fraction is calculated as a function of temperature which the alloy is quenched to. The example also shows how Cr content in the alloy influences M_s and M_{90} after intercritical annealing.

REFERENCE

Harris, William J, and Morris Cohen. 1949. "Stabilization Of The Austenite-Martensite Transformation." *Transactions of the American Society for Metals, AIME* 180: 447–70.

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

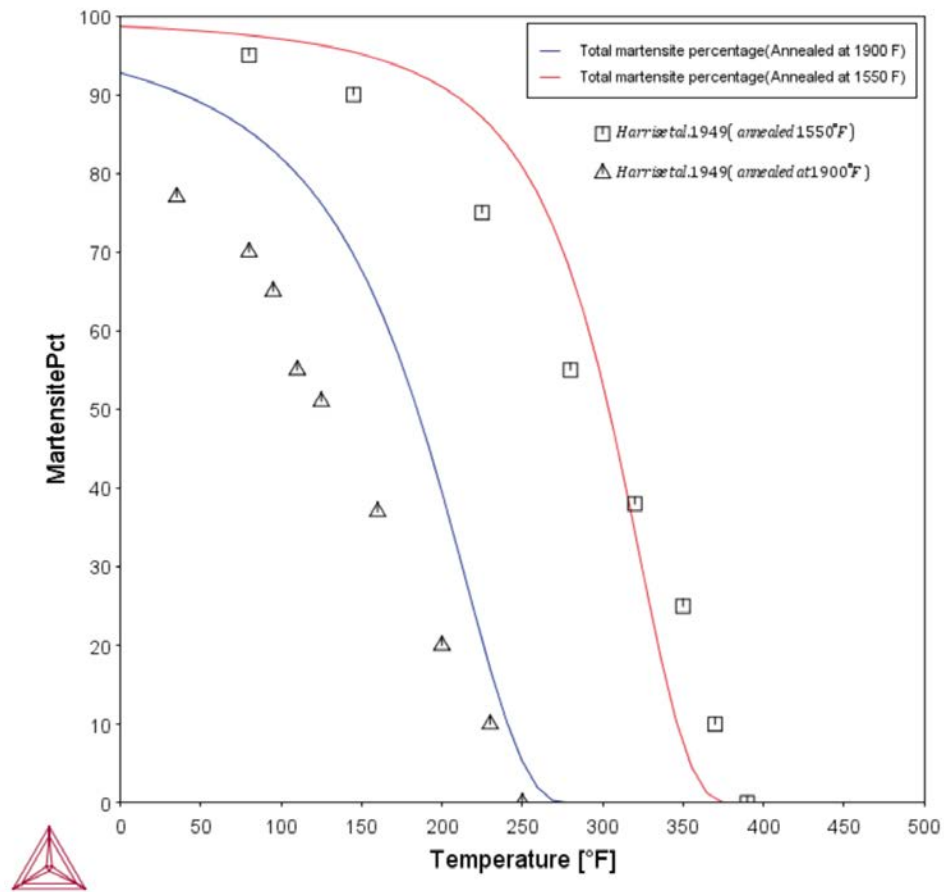
- Folder: Property models >Steel
- File name: *PM_Fe_01_Fe-Cr-C_martensite_intercritical_annealing.tcu*



Also see our [website](#) and [YouTube channel](#) for tutorial videos related to the Property Model Calculator.

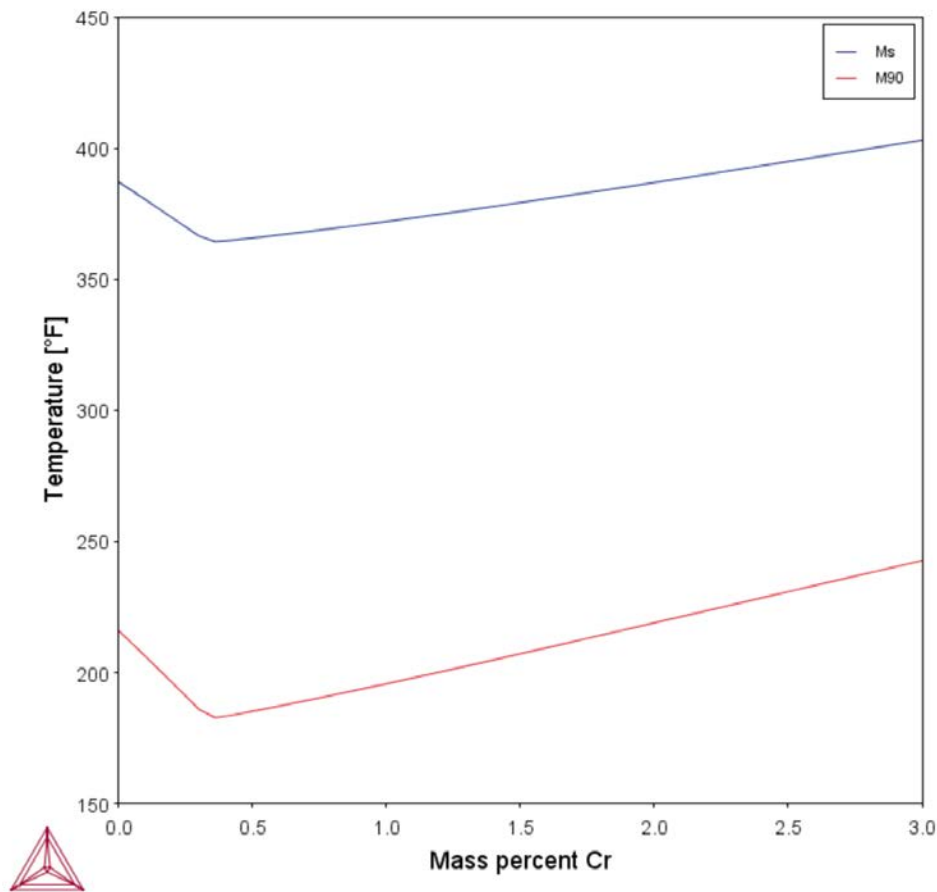
PLOT RESULTS

Transformation curves



The transformation curves plot showing Fe-Cr-C martensite with intercritical annealing.

Ms-Mf



PM_Fe_02: Fe-Mn Martensite Morphologies



To run calculations with the **Steel models** (martensite and pearlite) requires a valid maintenance license plus licenses for both the TCFE9 and MOBFE4 databases.

The example uses the Property Model Calculator with the **Martensite Temperatures** model. It shows the Ms temperatures of different types of martensites: lath, plate, and ϵ (hcp), compared with experimental ϵ Ms values.

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

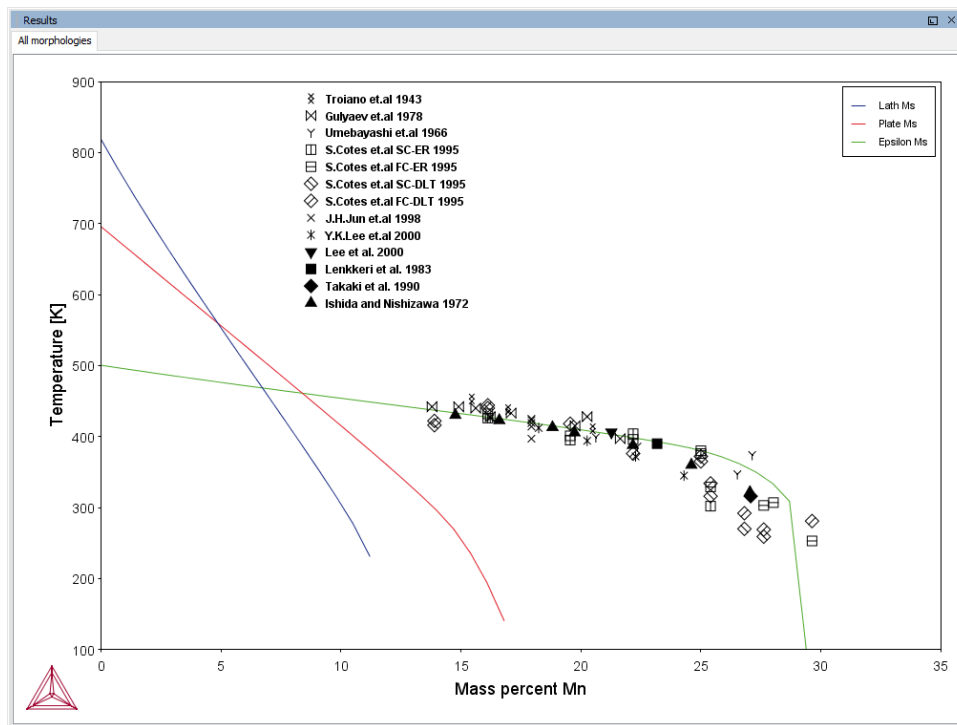
- Folder: Property Models>Steel
- File name: *PM_Fe_02_Fe-Mn_martensite_morphologies.tcu*



Also see our [website](#) and [YouTube channel](#) for tutorial videos related to the Property Model Calculator.

PLOT RESULT

All morphologies



A diagram showing all the Ms temperatures of different types of martensite morphologies (lath, plate and epsilon (hcp)) compared with experimental epsilon Ms values.

PM_Fe_03: Fe-C-Mn Pearlite



To run calculations with the **Steel models** (martensite and pearlite) requires a valid maintenance license plus licenses for both the TCFE9 and MOBFE4 databases.

The example uses the Property Model Calculator with the **Pearlite** model.

The example shows how to calculate pearlite growth rate, lamellar spacing, and times of start (2% transformation) and finish (98% transformation) as functions of isothermal heat treating temperature in an Fe-0.69C-1.80Mn alloy (mass %). With *maximize growth rate* set as the *criterion*, the model gives maximal growth rate and minimal lamellar spacing. With *optimal pearlite* as the *pearlite mode*, the model optimizes partitioning of substitutional alloying element(s) (Mn in this example) according to the criterion, which realizes a smooth transition between ortho-pearlite at high temperature and para-pearlite at low temperature.

REFERENCE

Razik, N.A, G.W. Lorimer, and N Ridley. 1974. "An Investigation of Manganese Partitioning during the Austenite-Pearlite Transformation Using Analytical Electron Microscopy." Acta Metallurgica 22 (10): 1249–58. doi:10.1016/0001-6160(74)90138-2.

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

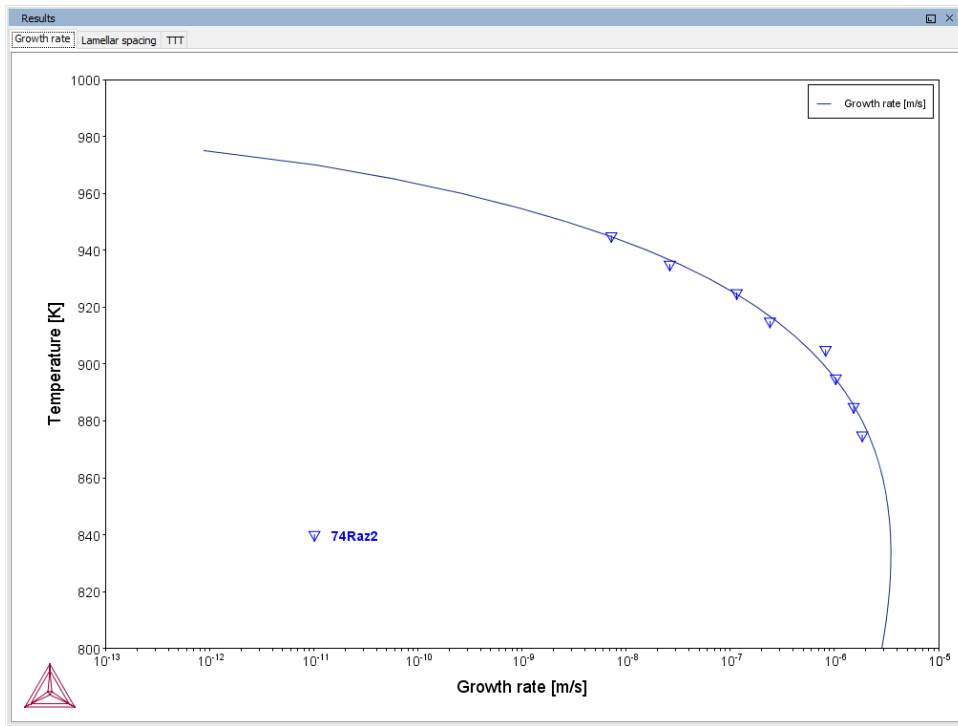
- Folder: Property Models>Steel
- File name: *PM_Fe_03_Fe-C-Mn_Pearlite.tcu*



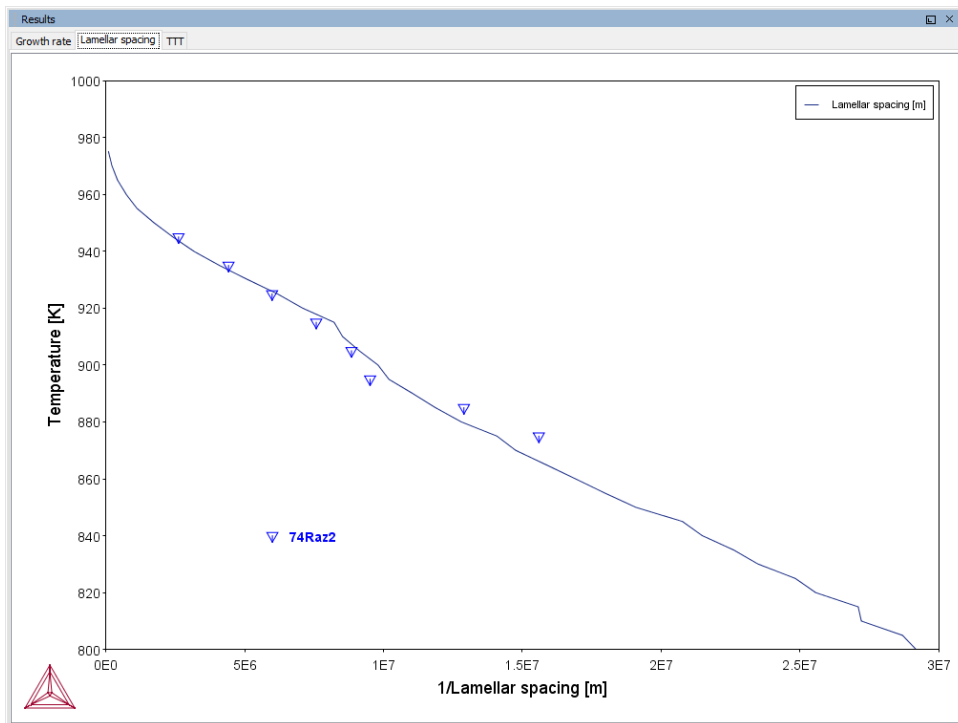
Also see our [website](#) and [YouTube channel](#) for tutorial videos related to the Property Model Calculator.

PLOT RESULTS

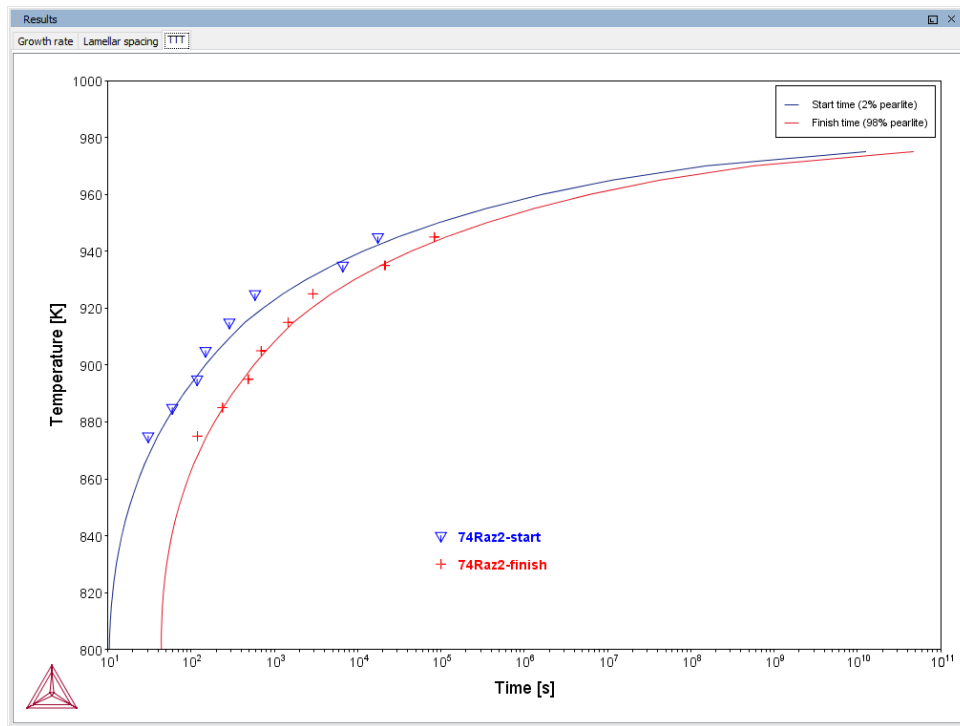
Growth Rate



Lamellar Spacing



TTT



The TTT (time-temperature-transformation) diagram showing times of start (2% transformation) and finish (98% transformation) as functions of isothermal heat treating temperature in an Fe-0.69C-1.80Mn alloy (mass %).

Process Metallurgy Examples Collection



The Process Metallurgy Module works with TCOX8 and newer versions of the database. The current version of the database is TCOX9.



All other users can test the module with the included OXDEMO database, which is limited to these elements: Al, C, Ca, Fe, O, S, and Si. For more information about this and other products [visit our website](#).



["About the Examples " on page 23](#)

PMET_01: Basic Oxygen Furnace (BOF)



This example does not require a license to run the simulation. It works with both the TCS Metal Oxide Solutions Database (TCOX versions 8 and 9 and newer) as well as the free OXDEMO database.

The example uses the **Process Metallurgy Calculator** to demonstrate a simplified steelmaking process in a Basic Oxygen Furnace (BOF).



The real-world BOF process is highly exothermic and needs adiabatic calculations. These are not available with the current version of the Process Metallurgy Module.

It is recommended you open the example project file and watch the companion video. The video walks you through setting up the material groups as well as analyzing the results.



You can open the example project file from Thermo-Calc **Help → Example Files → Process Metallurgy → PMET_01_Basic_Oxygen_Furnace.tcu**.



This example is included as a tutorial on our [website](#) and our [YouTube](#) channel.

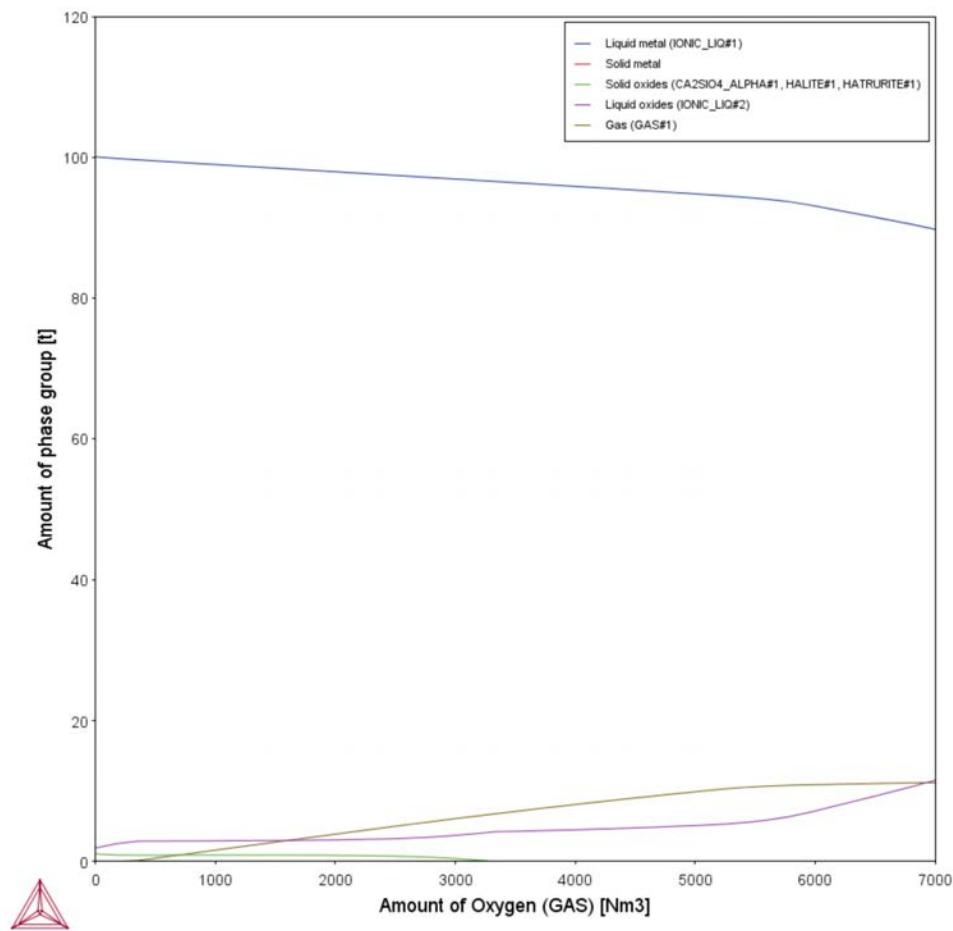
In general, the steps to set up this simulation are described in "[Defining the Process Metallurgy Calculator](#)" on page 164. After setting up the steel, slag and gas system, you can generate various plots to analyze the results. Below is a brief summary of this analysis.

- ▶ See "[Phase Groups](#)" on [page 158](#) for details about how the Process Metallurgy Module plot labels are grouped into the *liquid metal*, *solid metal*, *solid oxides*, *liquid oxides* and *gas* phases.

For this example, a **One axis** calculation type is used for all plots. The *Grid Definition* settings for these plots are also set on the Process Metallurgy Calculator:

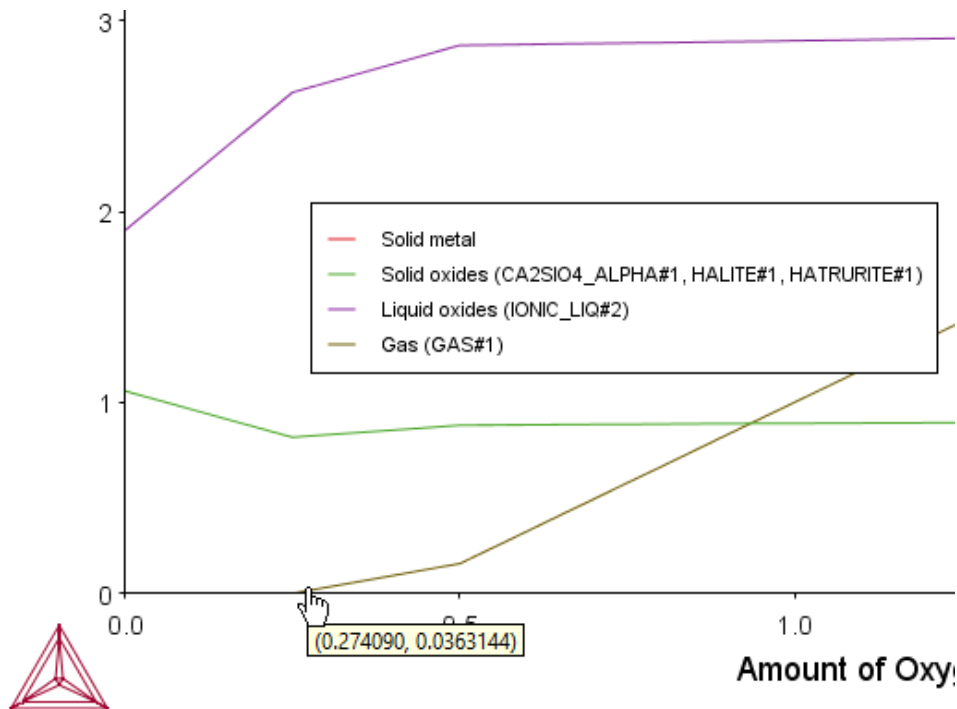
- Quantity: Amount of Oxygen (GAS)
- Stepping 0 min to 10 max with 40 steps

Amount of Phase Groups



After the plot is generated, by default you can see the **Amount of phase group** is plotted on the Y-axis as a function of the quantity plotted on the X-axis, in this case the **Amount of Oxygen (GAS)**.

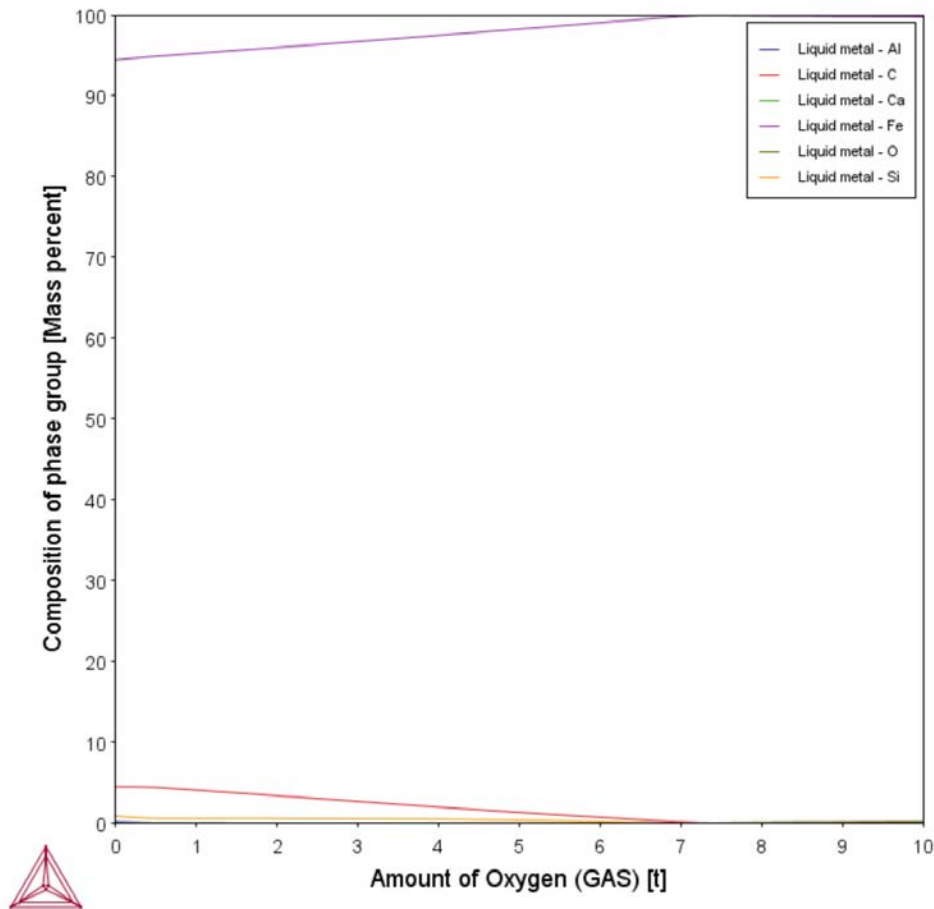
Zooming into the low gas amount (see below), it can be seen that the evolution of the gas phase is retarded. The reason is that the oxygen gas first oxidizes some of the silicon dissolved in the steel to form silicon dioxide (SiO_2). Only when the silicon content in the steel has dropped below a certain level can the oxygen gas burn away the carbon dissolved in the steel to form a carbon monoxide (CO)-rich gas phase.



These reactions can be investigated in more detail with different plots, so we will do that.

Composition of Liquid Metal

For the next plot, you define the following on a Plot Renderer, which you add to the Process Metallurgy Calculator. Keep the X-axis setting. For the Y-axis, choose **Composition of a phase group, Liquid Metal, All elements**.

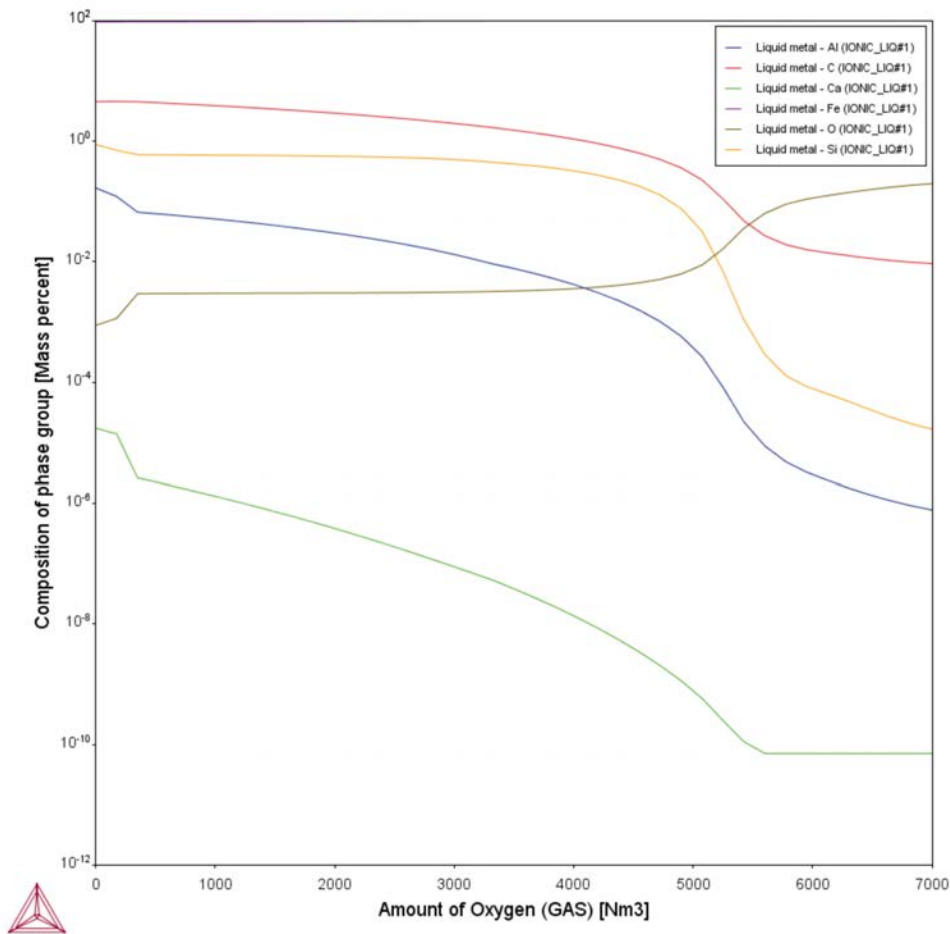


In the plot (that uses a linear axis) the reduction of the carbon content can be clearly seen. This reduction of the carbon content is what is termed “steelmaking”. The hot metal coming from the blast furnace has a very high carbon content of typically 4.5 wt%. If it is left to solidify without lowering the carbon content, it will be extremely brittle and be unfit for rolling or forging.

Other changes in steel chemistry occurring in the BOF can be made visible by changing the Y-axis type from linear to logarithmic.



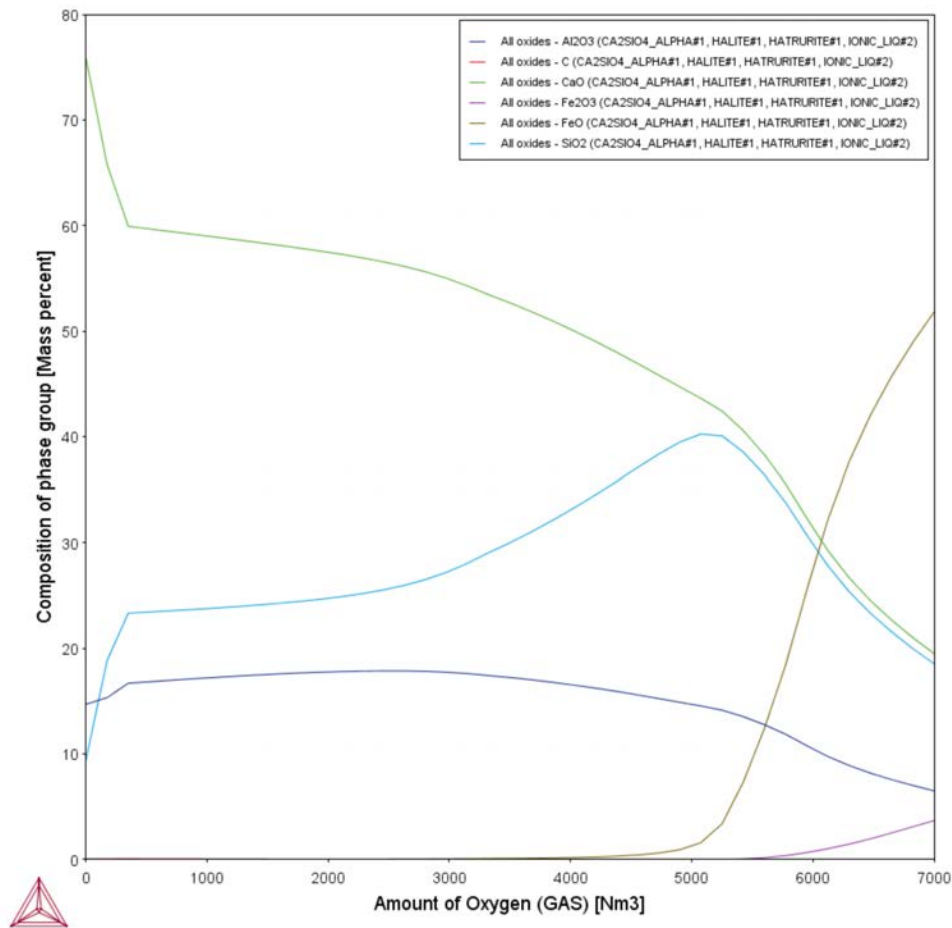
In the example project file only the logarithmic 10 version of the plot is included.



Now you can see the removal of the elements from the liquid steel in the following order: first calcium, then aluminium, then silicon and finally carbon (Ca, Al, Si and C) according to their position on the Ellingham diagram.

Composition of Liquid Slag

Add another Plot Renderer and define the following. Keep the X-axis setting. For the Y-axis, choose **Composition of a phase group, Liquid Oxides, All components**.



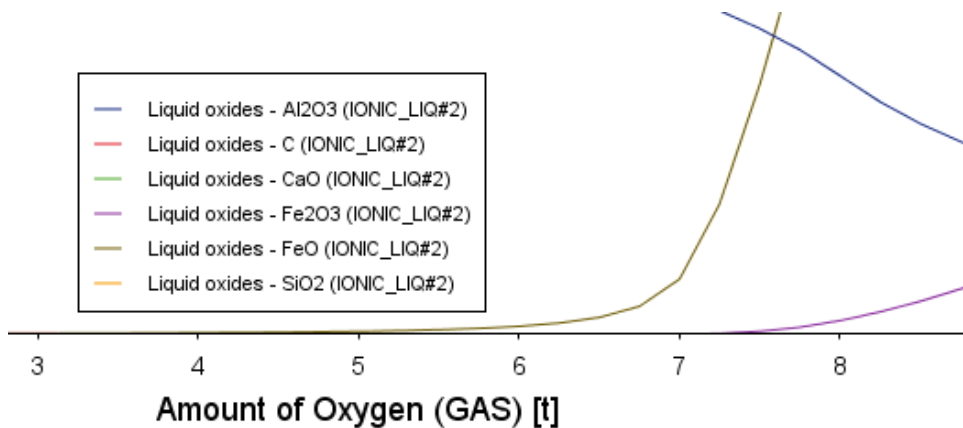
This plot shows how the liquid slag composition changes as a function of the amount of oxygen added to the BOF.

At first, the SiO_2 content of the slag rises sharply. This is due to the initial oxidation of the silicon dissolve in the hot metal. The SiO_2 that is formed combines with the slag and increases its SiO_2 content.

This increased SiO_2 content reduces the liquidus temperature of the slag and, as you can see in the first plot, thereby increases the amount of liquid slag and reduces the amount of solid oxides. This is also exactly what happens in reality.

On further addition of oxygen to the liquid steel, the silicon dioxide (SiO_2) content in the slag increases further and further as more silicon is oxidized and combines with the slag. At the same time the oxygen partial pressure in the steel slowly increases. After about 6 tonnes of oxygen have been added to the system, the oxygen pressure is high enough to start oxidizing the steel itself.

The slag quickly becomes rich in iron oxide (FeO). When this starts happening, the steelmaking process is complete and the steel is ready to be tapped into a ladle for further steel refining.



PMET_02: Ladle Furnace



This example does not require a license to run the simulation. It works with both the TCS Metal Oxide Solutions Database (TCOX versions 8 and 9 and newer) as well as the free OXDEMO database.

The example uses the **Process Metallurgy Calculator** to represent a simplified steel refining process in a ladle furnace (LF). It introduces you to the workflow of the Process Metallurgy Module. It is recommended you open the example project file and watch the companion video. The video walks you through setting up the material groups as well as analyzing the results.



You can open the example project file from Thermo-Calc **Help** → **Example Files** → **Process Metallurgy** → **PMET_02_Ladle_Furnace.tcu**.



This example is included as a tutorial on our [website](#) and our [YouTube](#) channel.

In general, the steps to set up this simulation are described in "[Defining the Process Metallurgy Calculator](#)" on page 164. After setting up the steel, slag and gas system, you can generate various plots to analyze the results. Below is a brief summary of this analysis.



See "[Phase Groups](#)" on page 158 for details about how the Process Metallurgy Module plot labels are grouped into the *liquid metal*, *solid metal*, *solid oxides*, *liquid oxides* and *gas* phases.

The material saved for this example, *Steel_LF*, could be a typical, but simplified composition of a fully killed SAE 1040 grade steel. The sulfur content, however, is too high for most final applications and must be reduced. Sulfur is usually removed from liquid steel in a ladle furnace using a calcium oxide-rich slag.

In this example, we want to find a slag composition that efficiently desulphurizes the steel. For this particular calculation we choose not to define a constant amount of slag but instead use absolute amounts of components. To do this, we set the **Input type** for the **Slag** material group to use **Absolute amount**. After saving this composition, it becomes the slag material for this example, *Slag_LF*.

| Material: | Slag | Slag_LF | | |
|-----------------------------------------------------|-----------------|-----------|--------|------|
| Amount: | Kilogram | 2500.0 | | |
| Input type: | Absolute amount | Component | | |
| <input type="checkbox"/> Hide composition | | | | |
| <input type="checkbox"/> Normalize to total of 100% | | | | |
| + | - | CaO | 2000.0 | 80.0 |
| + | - | Al2O3 | 250.0 | 10.0 |
| + | - | SiO2 | 250.0 | 10.0 |
| Total: | | 2500.0 | 100.0 | |



For this example, the gas phase is not considered, which is why the Gas material group has been removed in the example project. This does not mean that no gas phase is allowed to form; it simply means that no gas phase is used to set the calculation conditions.

For this example, a **Grid** calculation type is used for all plots. The *Grid Definition* settings for these plots are also set on the Process Metallurgy Calculator:

| Quantity | Min | Max | Number of steps |
|-----------------------------------|-----|--------|-----------------|
| Amount of Al2O3 in Slag_LF (SLAG) | 0.0 | 1000.0 | 10 |
| Amount of SiO2 in Slag_LF (SLAG) | 0.0 | 1000.0 | 10 |



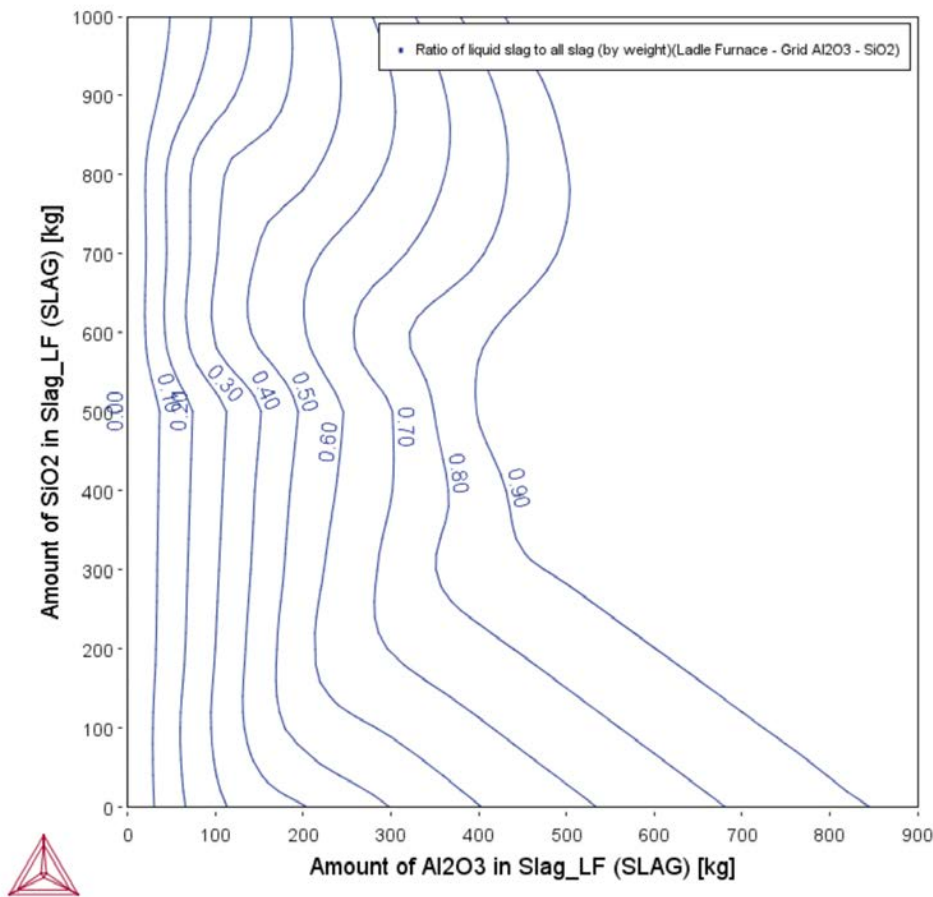
Leave the number of calculation steps at 10 for both axes in order to shorten the calculation time. With this setting, the calculation should be completed in just under one minute. The number of steps could be increased to maybe 30 x 30 for higher resolution of the results, but this increases the calculation time significantly.

Fraction of Liquid Slag



In the example project file only the *Ratio of liquid slag and sulfur in liquid steel* contour plot is included.

We want to understand whether our slag phase is liquid or not. To create the plot below, add a Plot Renderer node with a **Contour** plot and choose **Fraction of liquid slag** as the **Z-axis variable**. Set the interpolation as **50 x 50** and click **Perform**.



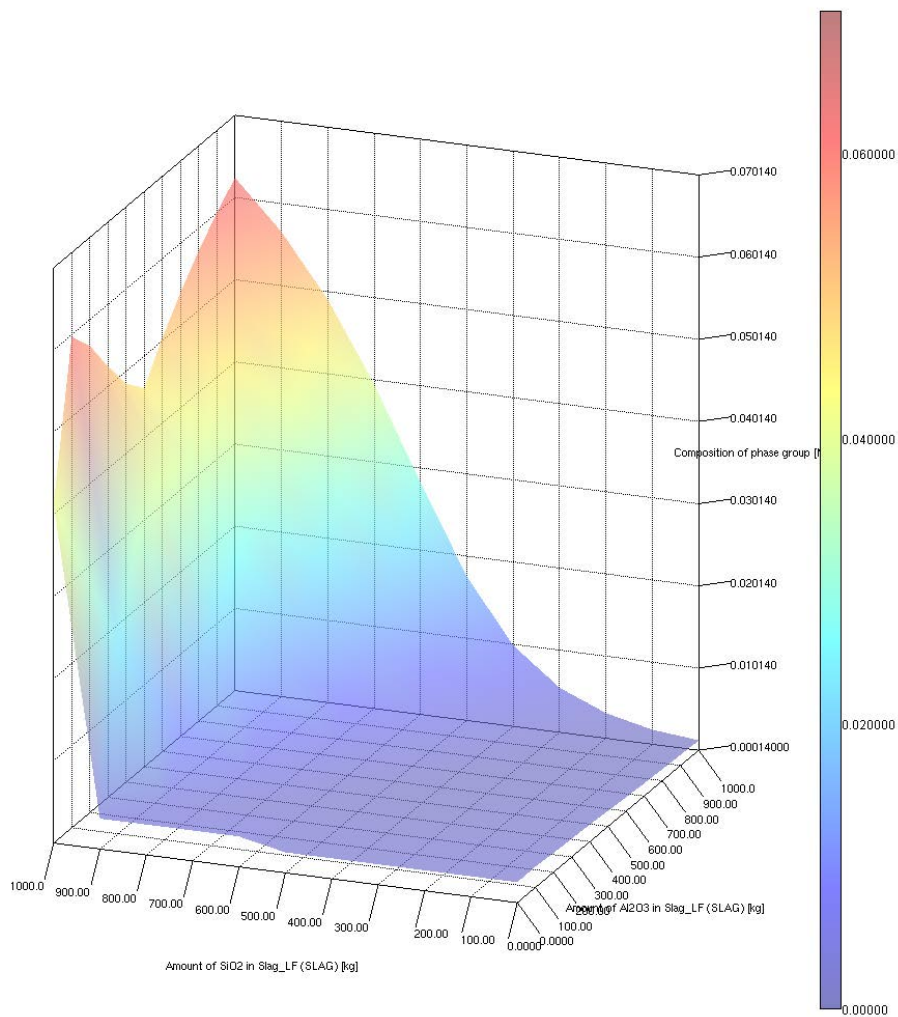
The plot shows that for low amounts of aluminium oxide (Al_2O_3) and silicon dioxide (SiO_2), almost no liquid slag is present. Process metallurgists refer to this as a *hard slag*.

Such a hard slag is in fact just solid oxide phases that passively float on the liquid steel. It does not react with the liquid steel for kinetic reasons and therefore does not desulfurize the steel.

Practical slag compositions are limited to the top, right field above the “fraction liquid slag = 0.9” contour line. Only here a liquid slag phase is present that can flow and can mix and react with the steel.

Next we are interested in the ability of the slag phase to remove sulfur (s) from the liquid steel.

Sulfur in Liquid Steel



Refer to the *Sulfur in liquid steel* 3D plot included with the example. The red colors in the upper right-hand corner at high SiO_2 and Al_2O_3 content show that the steel contains high amounts of sulfur.

This means that only a little of the sulfur in the liquid steel partitioned into the slag phase and the slag phase has a poor capacity to take up sulfur.

The blue colors in the lower left-hand corner indicate that the liquid steel contains only very low amounts of sulfur, so this indicates a slag composition that is effective at removing sulfur, or in other words, has a high sulfur capacity.



The performed calculations assume thermodynamic equilibrium. As shown in the previous plot, there is almost no liquid slag phase present in the lower left corner at low SiO_2 and Al_2O_3 content. This means that thermodynamic equilibrium would not be achieved due to the very slow kinetics of the reaction between the liquid steel and the solid oxides.

Ratio of Liquid Slag and Sulfur in Liquid Steel

Refer to the *Ratio of liquid slag and sulfur in liquid steel* contour plot included with your example. This is two plots combined into one contour plot. If you created the above *Fraction of Liquid Slag* contour plot, this plot is created simply by adding another set of axes and then defining the Z-axis.

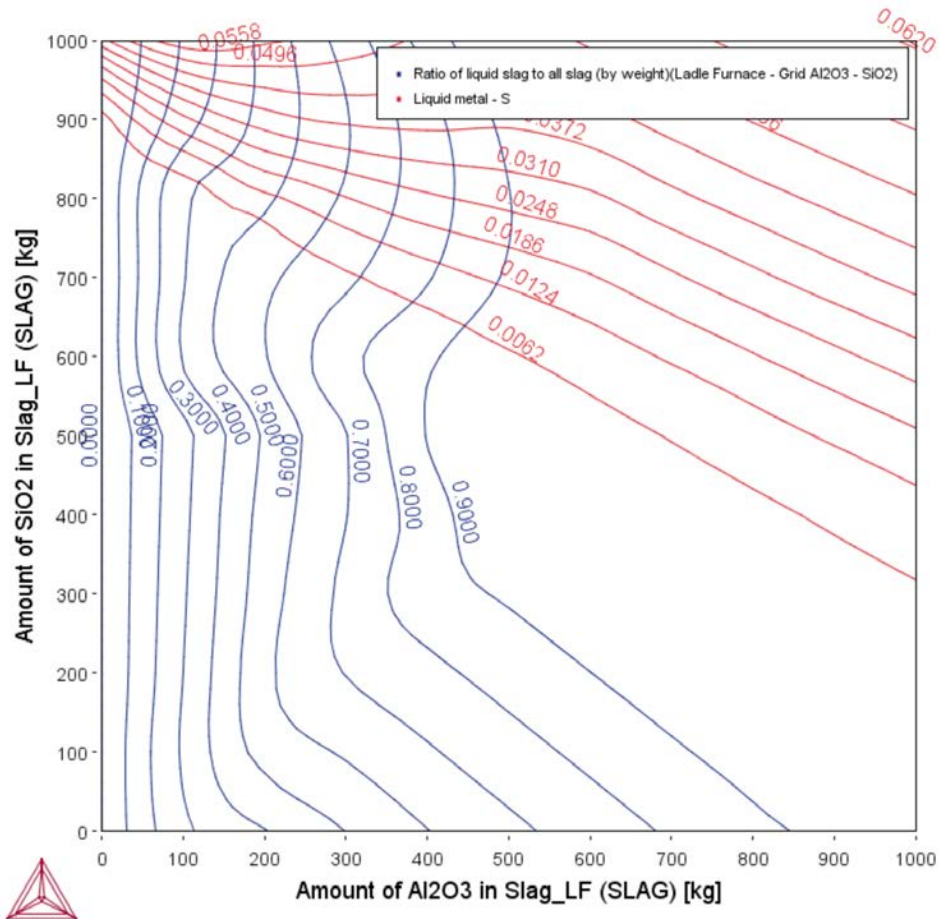
Z-axis

Axis variable: Composition of phase group Liquid metal S

Axis type: Linear

Limits: 0.0 to 1.0 step 0.1 ☒ Automatic scaling

Combining the information contained in the two plots results in an optimum slag composition in a narrow composition band. To smooth the contours, Set the interpolation as **50 x 50**.



To map this optimal composition field one more plot can be generated by superimposing contour plots of sulfur content in the liquid steel and fraction of liquid slag.

Since we want to have at least 95% liquid slag, in the set of axis variables for **Fraction of liquid slag**, click to select the check box next to **Use custom contour values** and enter 0.95 in the field.

We also want to have less than 0.005% sulfur in the liquid metal, so also select the same check box for the other Z-axes and set the value of sulfur to 0.005. Click **Perform**.

Z-axis

Axis variable: Fraction of liquid slag

Axis type: Linear

Limits: 0.0 to 1.0 step 0.1 ☒ Automatic scaling

Contour values: 0.95 ☒ Use custom contour values

☒ ☒ ☒

X-axis

Axis variable: Amount of Al2O3 in Slag_LF (SLAG) Kilogram

Limits: 0.0 to 1.0 step 0.1 ☒ Automatic scaling

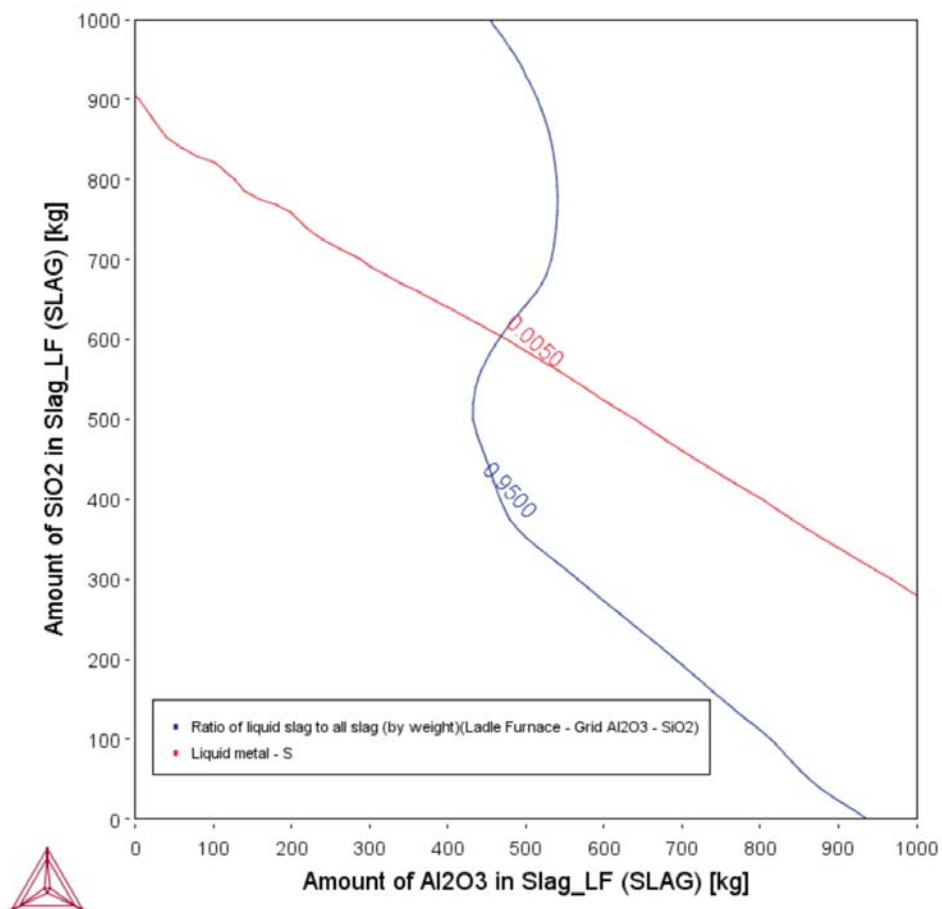
Z-axis

Axis variable: Composition of phase group Liquid metal S Mass percent

Axis type: Linear

Limits: 0.0 to 1.0 step 0.1 ☒ Automatic scaling

Contour values: 0.005 ☒ Use custom contour values



The optimal slag has a composition delimited by these two contour lines, so below the contour line for sulfur content in the liquid steel and above the contour line for fraction of liquid slag will be both fully liquid and effectively desulfurizes the steel.

PMET_03_Argon_Oxygen_Decarburization



This example does not require a license to run the simulation. It works with both the TCS Metal Oxide Solutions Database (TCOX versions 8 and 9 and newer) as well as the free OXDEMO database.

The example uses the **Process Metallurgy Calculator** to



You can open the example project file from Thermo-Calc **Help → Example Files → Process Metallurgy → PMET_03_Argon_Oxygen_Decarburization.tcu**.

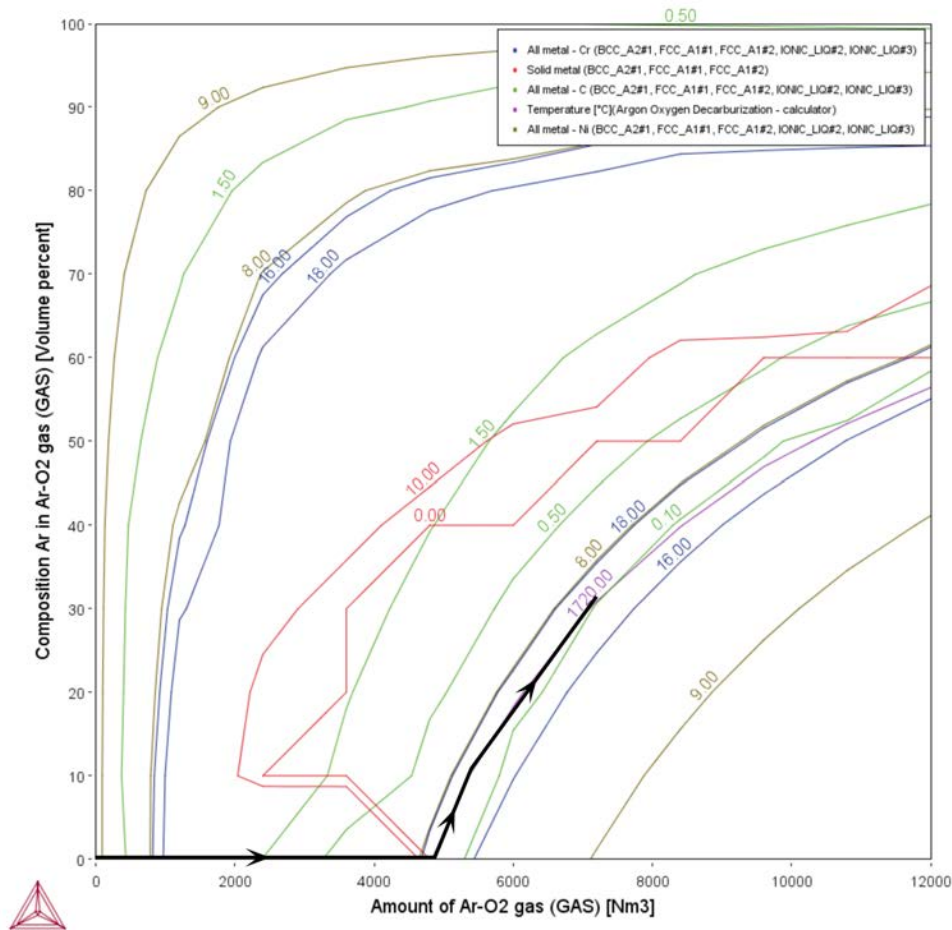


See the Process Metallurgy Module examples that are available as video tutorials on our [website](#) and our [YouTube](#) channel.



The example takes several minutes to run.

The Argon Oxygen Decarburization (AOD) process is a converter process applied in stainless steel making. In this process the oxidation of chromium in the steel melt needs to be prevented while carbon is oxidized. This is achieved by reducing the oxygen partial pressure by having a high Ar-content in the blowing gas. It is a highly exothermic process that requires adiabatic modeling. In this example the conversion of carbon-rich steel scrap is modeled together with additions of Ferronickel and Ferrochrome to a stainless steel.

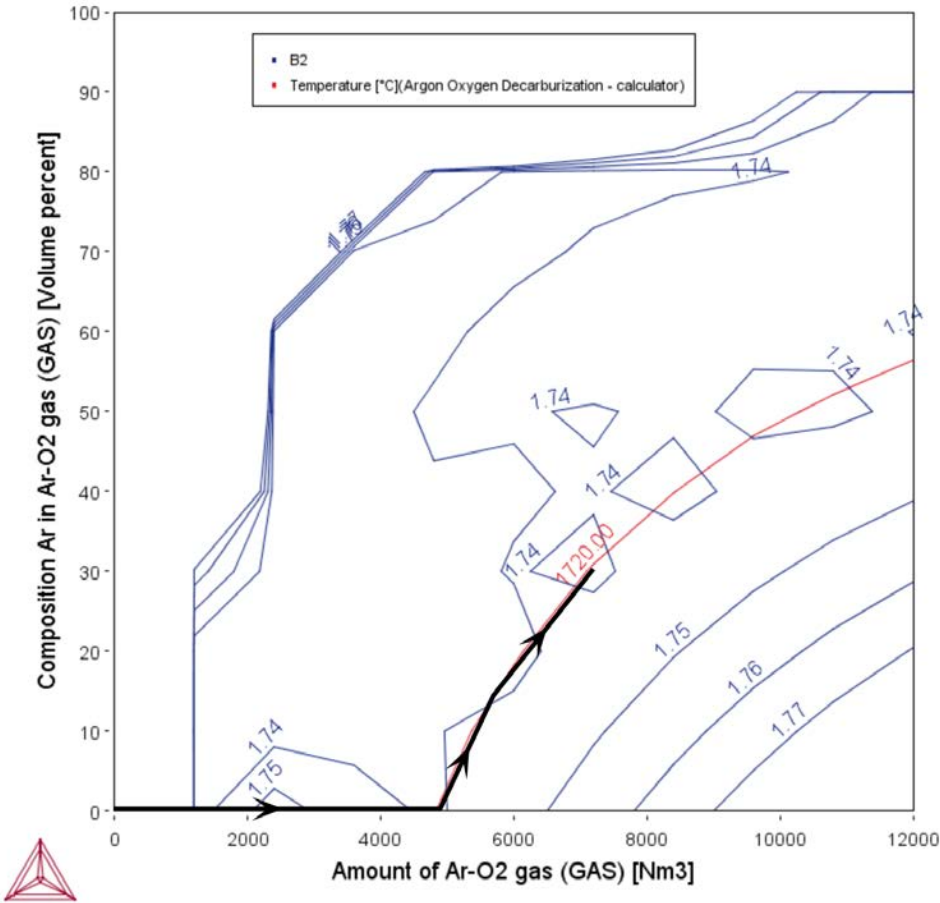


The AOD-process is characterized by an initially high O₂-content of the blowing gas, which is gradually replaced by Ar. The maximum temperature of the process is typically around 1720 °C. A grid plot of an adiabatic calculation is well suited to model the required simultaneous change of amount of gas and its composition during this process. The black line in the plot above indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

In principle, this plot could be used to control the blowing gas flow in a plant process. However, note that the simulation only considers a global gas phase, i.e. additional gas is added but never removed. This means that the given gas phase composition is an average one and not identical to the composition of the gas flowing in at each point in time. Additionally there is a certain impact on the resulting equilibria from the fact that all gas remains in the system and is not removed.

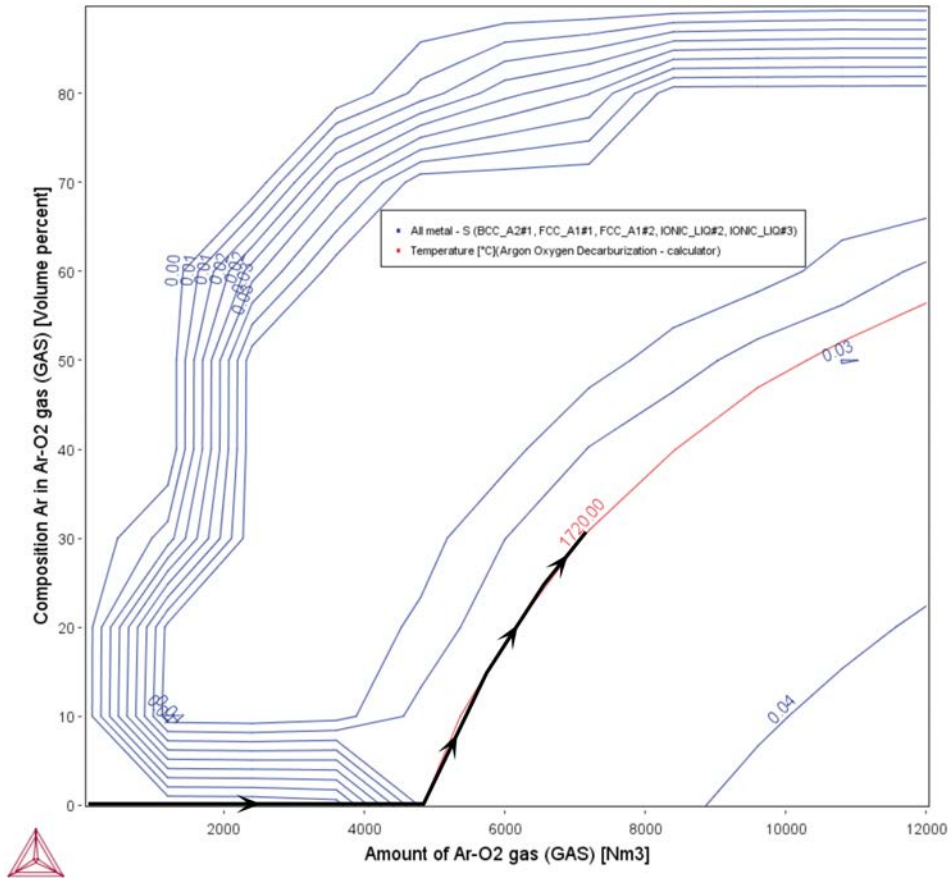
PLOTS

Slag Basicity



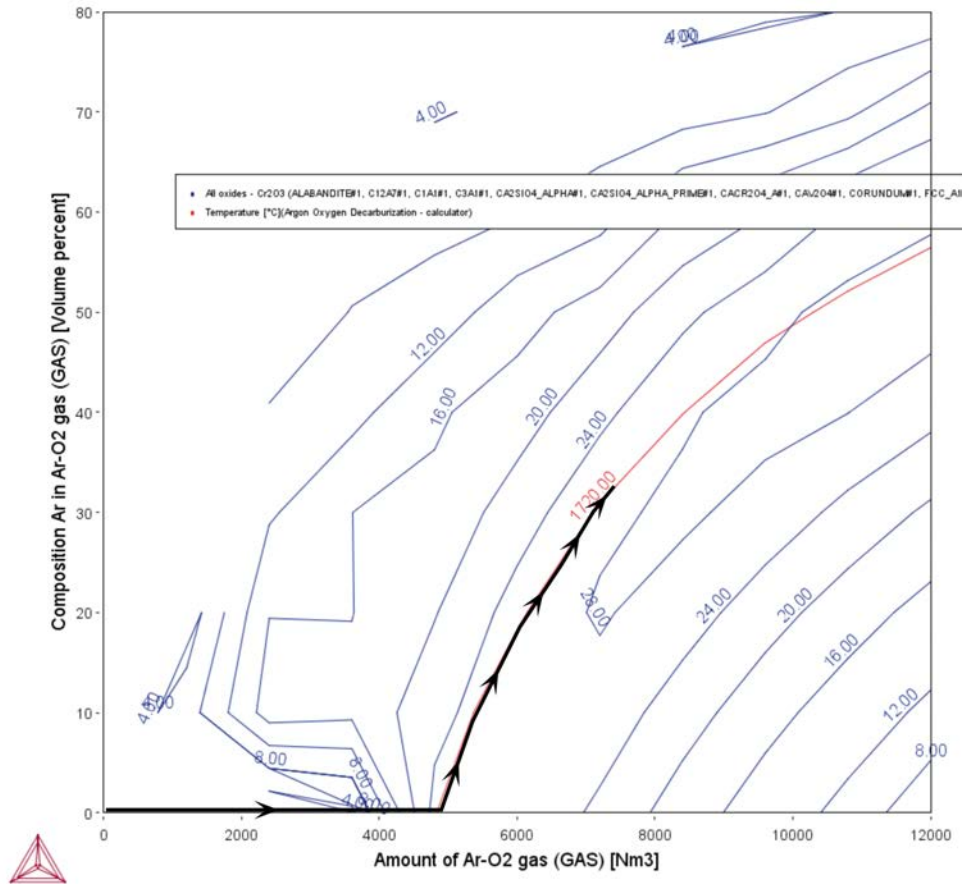
The Slag Basicity plot shows the basicity of the slag (which is a measure for the sulphur capacity of the slag). The process achieves a final basicity of 1.74 which is typical for an AOD-process. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

S Content in Steel



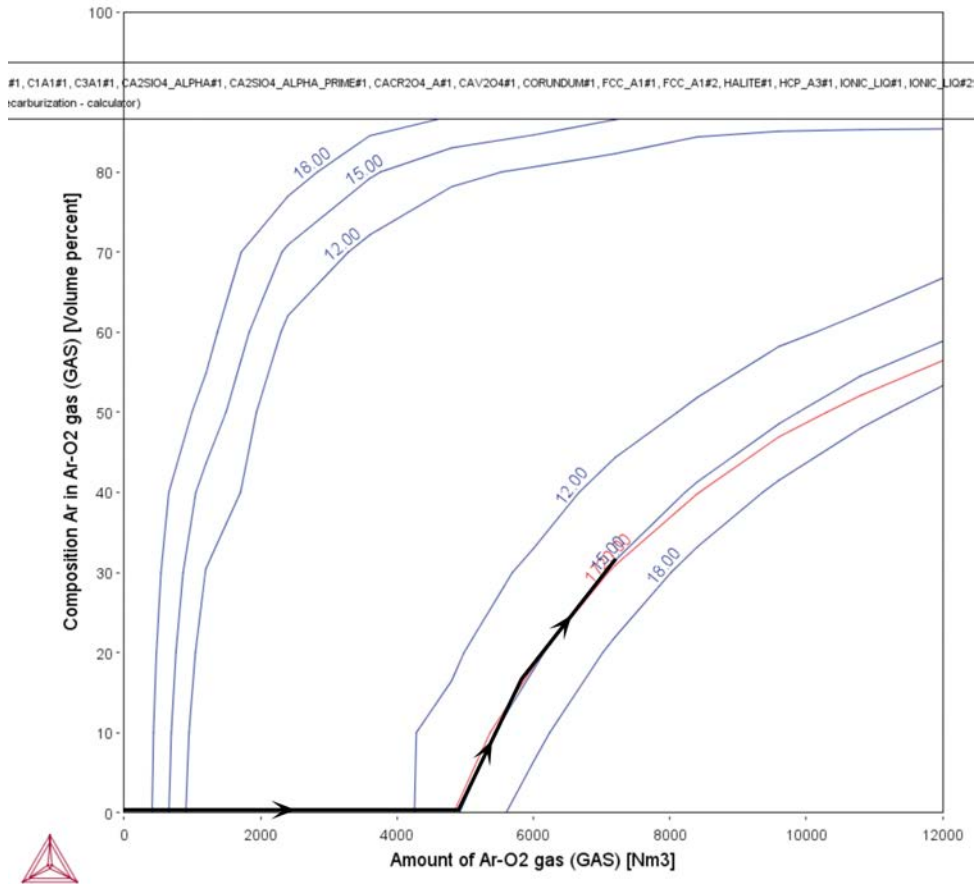
In the S Content in Steel plot, the sulphur content in the steel melt is slightly reduced during the process from 0.056% in the initial steel scrap to finally ca. 0.035%. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

Cr Content in Slag



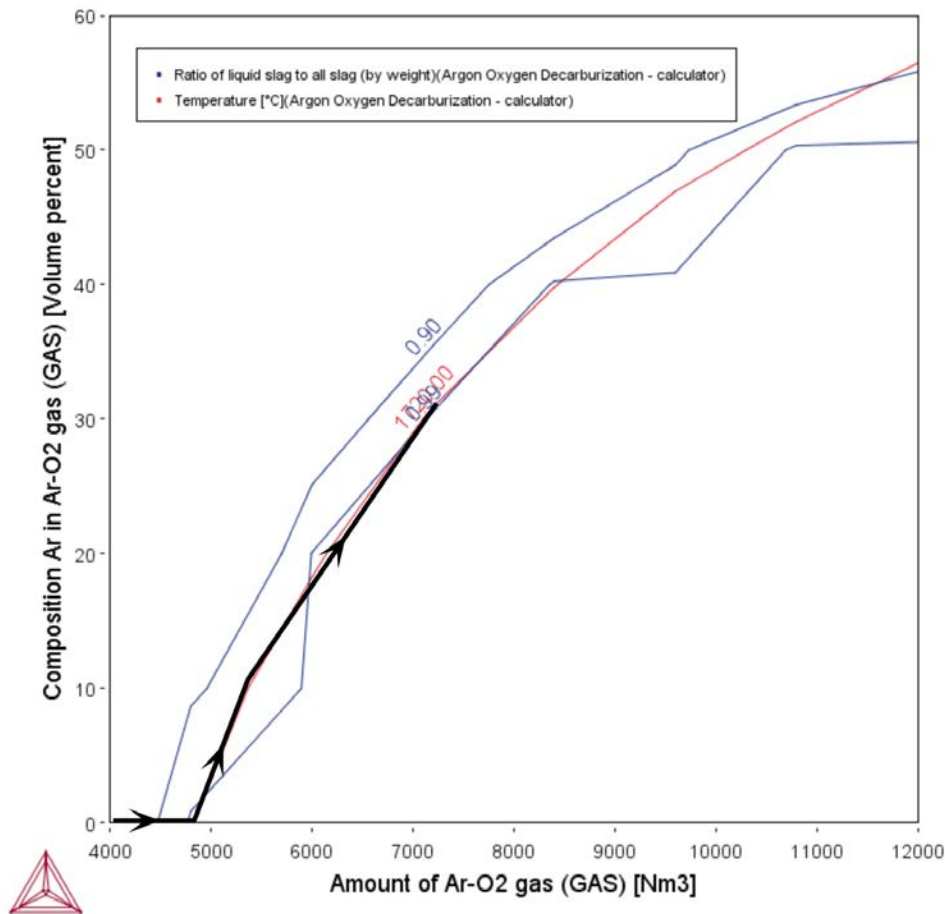
In the Cr Content in Slag plot, the Cr_2O_3 -content in the slag reaches at the end of the process ca. 26 wt-%. This is typical for the AOD-process and requires an additional Cr-recovery step after the conversion to reduce the loss of chromium. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

Amount of Slag



In the Amount of Slag plot, you can see that the process generates about 15 tons of slag in the total. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

Liquid Slag Fraction



In the Liquid Slag Fraction plot, you can see that towards the end of the process the slag is calculated to be mostly liquid. The black line in the plot indicates a possible process control path that finally leads to suitable alloy composition close to a X5CrNi 18-10 stainless steel.

Diffusion Module (DICTRA) Graphical Mode Examples



Examples using up to three elements are available to all users. The other examples require a Diffusion Module (DICTRA) license to calculate and plot results.

These examples use the **Diffusion Calculator**. All examples use demonstration database packages included with your installation no matter what licenses you have.

▶ ["About the Examples " on page 23](#)

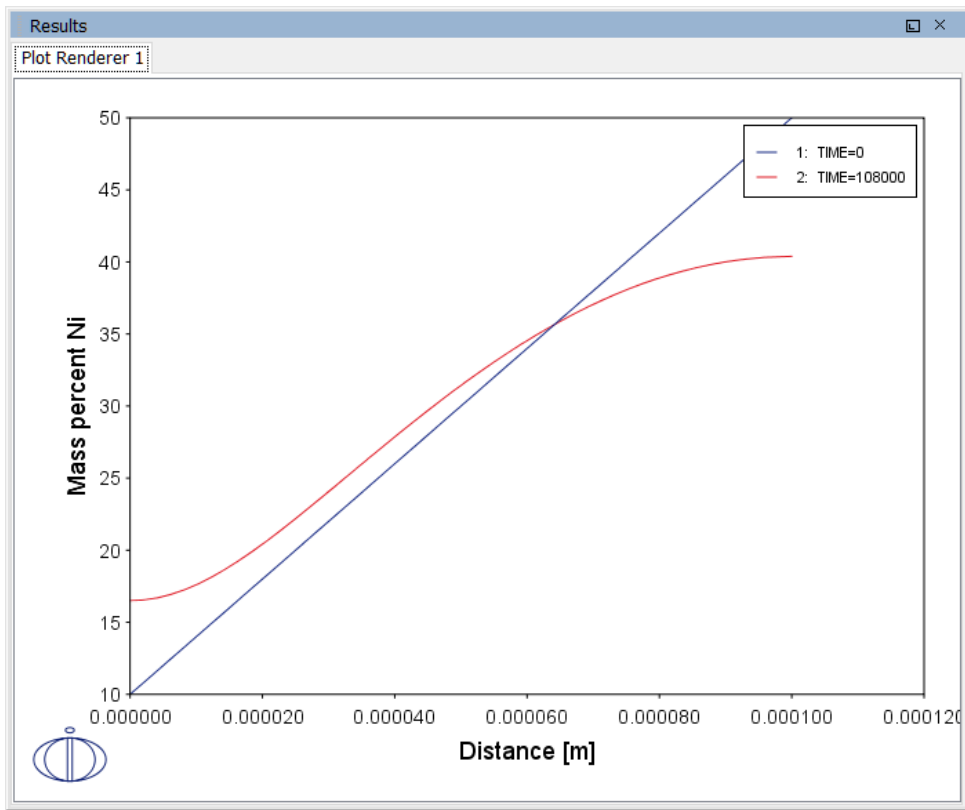
D_01 Homogenization of a Binary Fe-Ni Alloy

The single phase example simulates the diffusion of Fe and Ni at a temperature of 1400 K in a planar domain. At this temperature the material is fully austenitic, i.e. the only phase present is the so-called fcc (face centered cubic) phase. Initially, there is a linear variation in Ni going from 10 mass-% on the left-hand side to 50 mass-% on the right-hand side.



This example is available as a video tutorial on [our website](#) and [YouTube channel](#). In previous versions of the software (prior to 2017b) it is example 19.

Composition of Ni vs Distance



PROJECT FILE NAME

- Folder: Diffusion Module - DICTRA
- File name: *D_01_Diffusion_Single_Phase.tcu*



This example is part of the *Diffusion Module (DICTRA) Quick Start Guide* available to all users. A version of the example is also available for Console Mode.

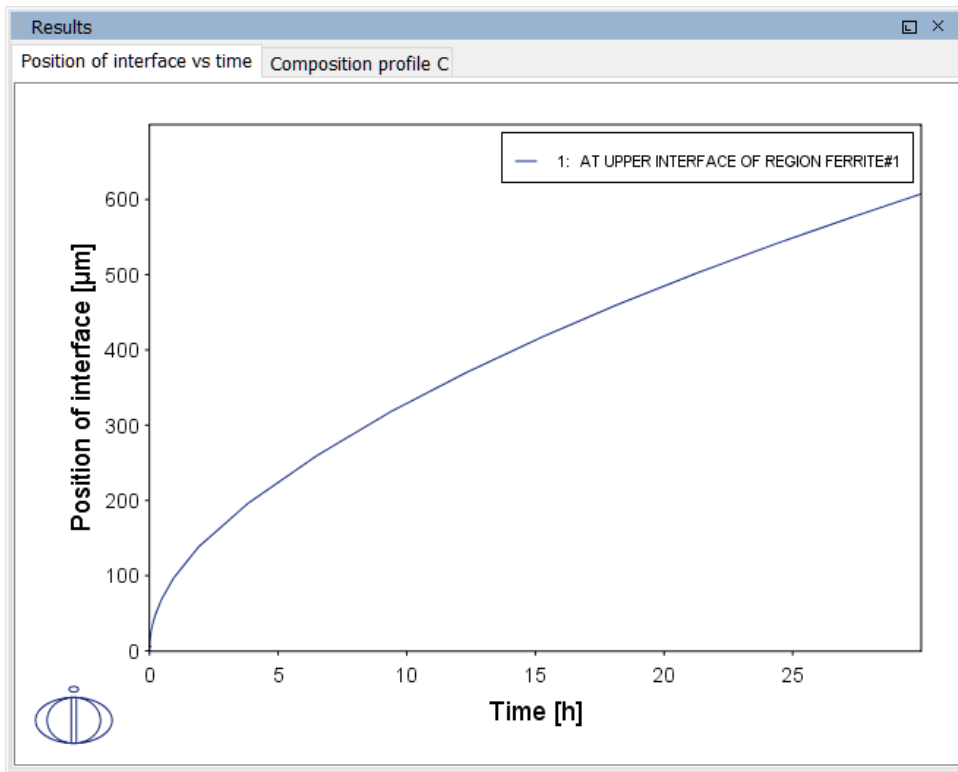
D_02 Ferrite(bcc)/Austenite(fcc) Transformation in a Binary Fe-C Alloy

The moving phase boundary example simulates the growth of ferrite (bcc) into austenite (fcc). The austenite is assumed to be initially homogeneous with the composition Fe-0.15 mass-% C. The transformation temperature is 1050 K. The initial thickness of the austenite is 2 mm and an initially very thin ferrite (1 nm) is also present at the start of the simulation.

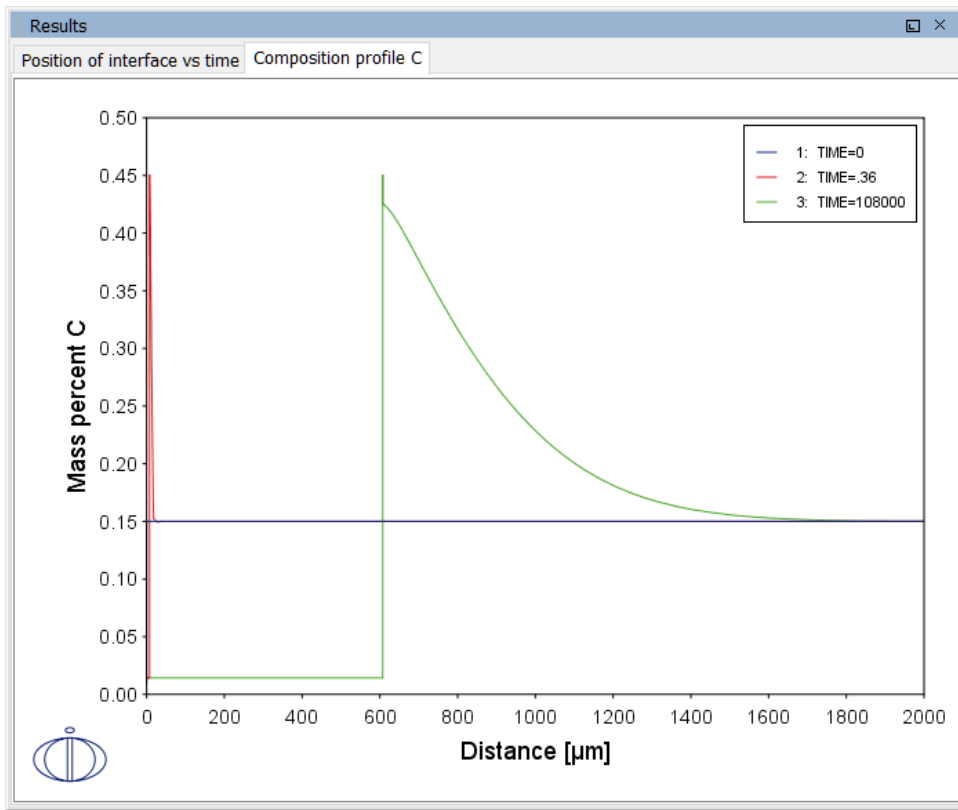


This example is available as a video tutorial on [our website](#) and [YouTube channel](#).

Position of interface vs time



Composition profile C



PROJECT FILE NAME

- Folder: Diffusion Module - DICTRA
- File name: *D_02_Diffusion_Moving_Boundary.tcu*



This example is part of the *Diffusion Module (DICTRA) Quick Start Guide* available to all users. A version of the example is also available for Console Mode.

D_03 Evolution of an Fe-Cr-Ni Diffusion Couple

The multiphase example simulates the evolution of an Fe-Cr-Ni diffusion couple during a 100 hour heat treatment at 1100° C (1373.15 K). Both end members of the diffusion couple are duplex ferrite plus austenite, but the majority phase is ferrite on the left-hand side and austenite on the right.

With this type of simulation it is assumed that the material is fully equilibrated at each grid point, i.e. the local phase fractions, phase compositions and so forth are obtained from an equilibrium calculation with the local overall composition as a condition.

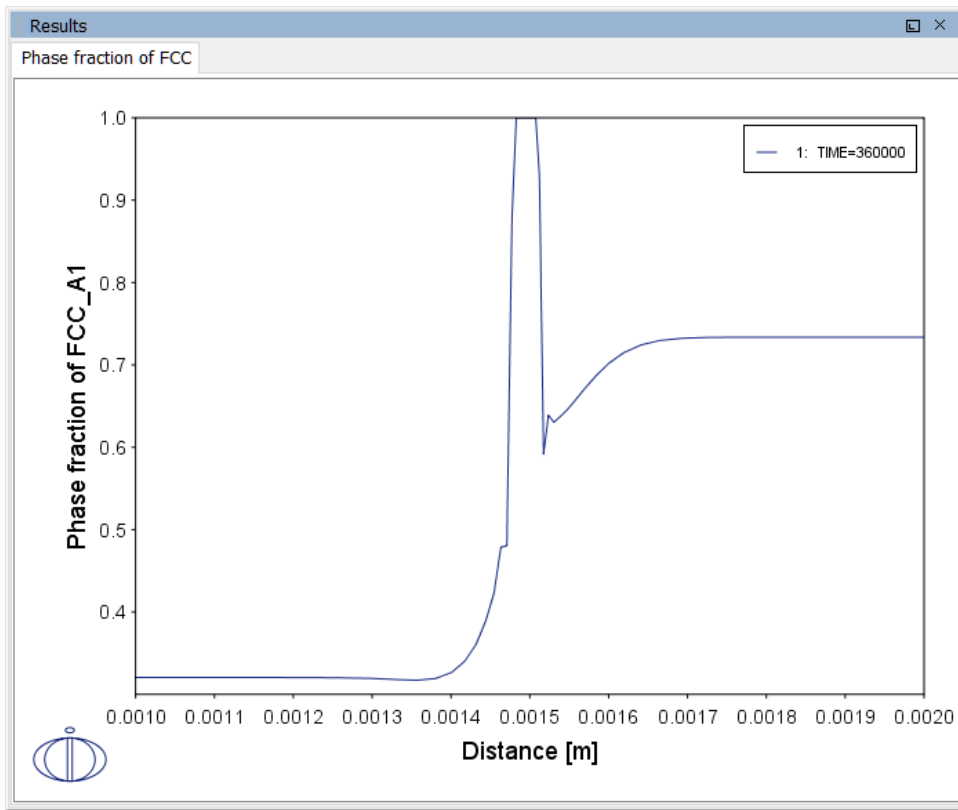
More details about the homogenization model for multiphase simulations can be found in Larsson and Engström (2006)¹ and Larsson and Höglund (2009)². Experimental data is from Engström (1995)³.

1. "A homogenization approach to diffusion simulations applied to $\alpha + \gamma$ Fe–Cr–Ni diffusion couples", *Acta Mater.*, 54 (9), pp. 2431–2439.

2. "Multiphase diffusion simulations in 1D using the DICTRA homogenization model", *Calphad*, 33 (3), pp. 495–501.

3. "Interdiffusion in multiphase, Fe-Cr-Ni diffusion couples", *Scand. J. Metall.*, 24(1), 12–20.

Phase fraction of FCC



PROJECT FILE NAME

- Folder: Diffusion Module - DICTRA
- File name: *D_03_Diffusion_Multiphase.tcu*

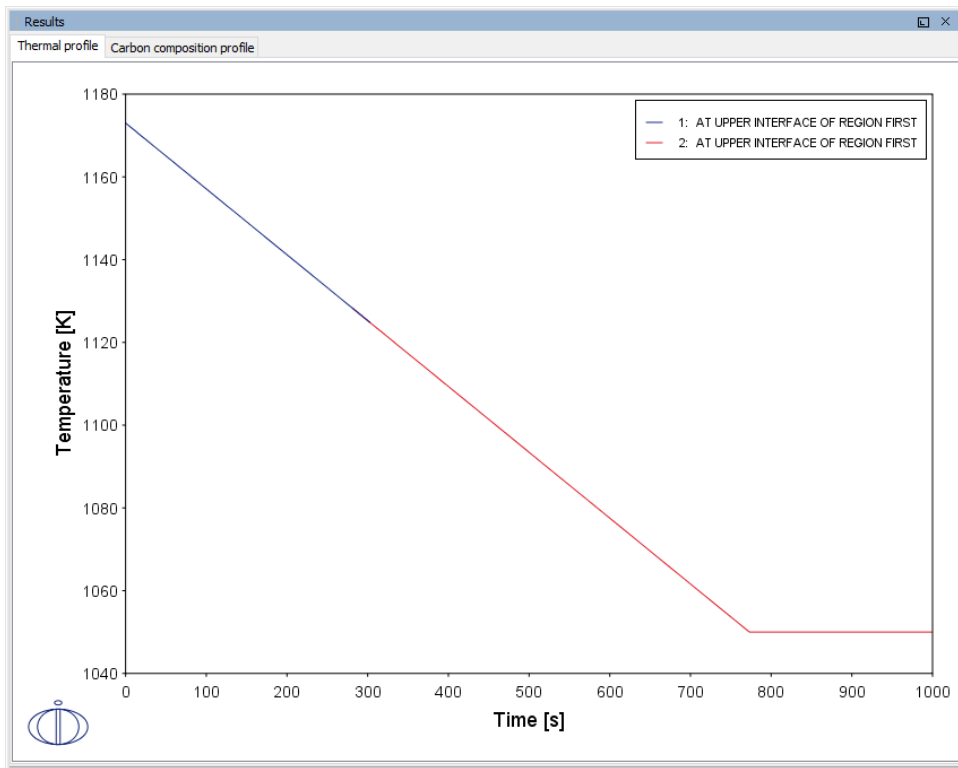


This example is part of the *Diffusion Module (DICTRA) Quick Start Guide* available to all users. A version of the example is also available for Console Mode.

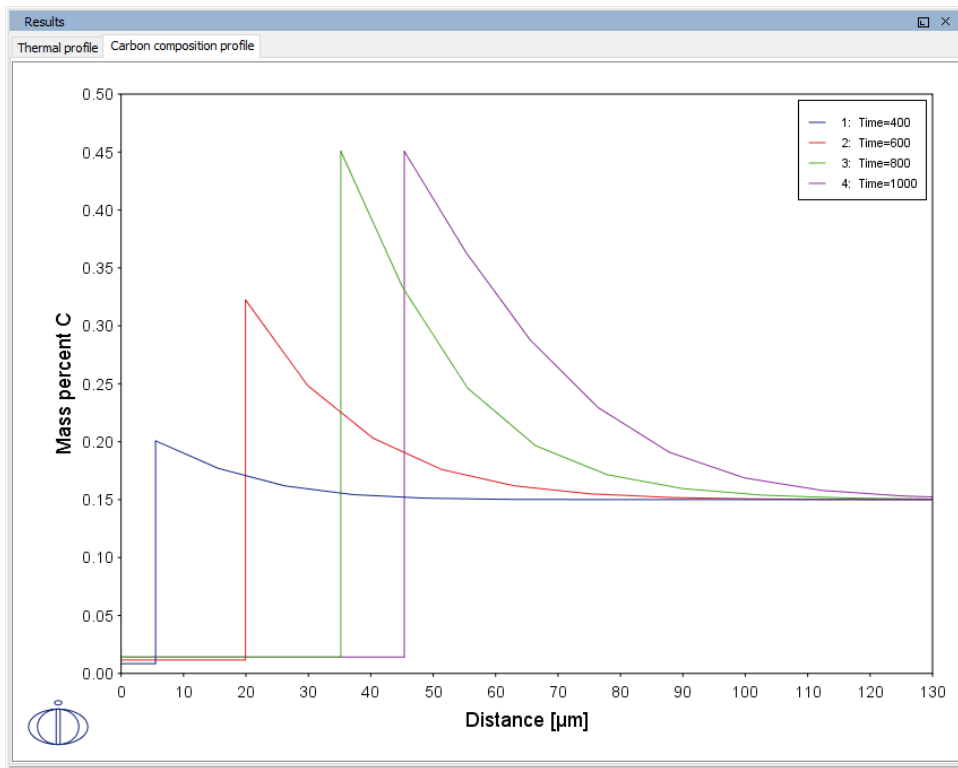
D_04 Fe-C Moving Boundary: Austenite to Ferrite

This example simulates the austenite to ferrite transformation in a Fe-0.01 mass% C steel during continuous cooling. The simulation starts at a temperature where only austenite is stable, ferrite nucleates and grows into the austenite during cooling in the two phase region. Plots of thermal and carbon composition profiles are generated.

Thermal profile



Carbon composition profile



PROJECT FILE NAME

- Folder: Diffusion Module - DICTRA
- File name: *D_04_Diffusion_Fe-C_Moving_Boundary_Austenite_to_Ferrite.tcu*

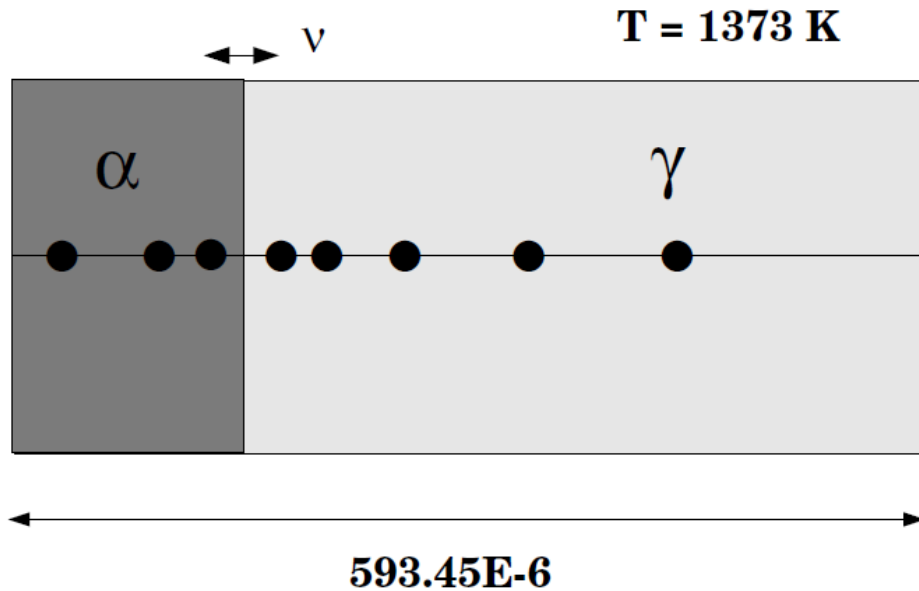


This example is available to all users.

D_05 $\gamma/\alpha/\gamma$ Diffusion couple of Fe-Ni-Cr alloys

This example demonstrates the evolution of a ternary Fe-Cr-Ni diffusion couple. A thin slice of ferrite (α phase) (38%Cr,0%Ni) is clamped between two thicker slices of austenite (γ phase) (27%Cr, 20%Ni). The assembly is subsequently heat treated at 1373 K.

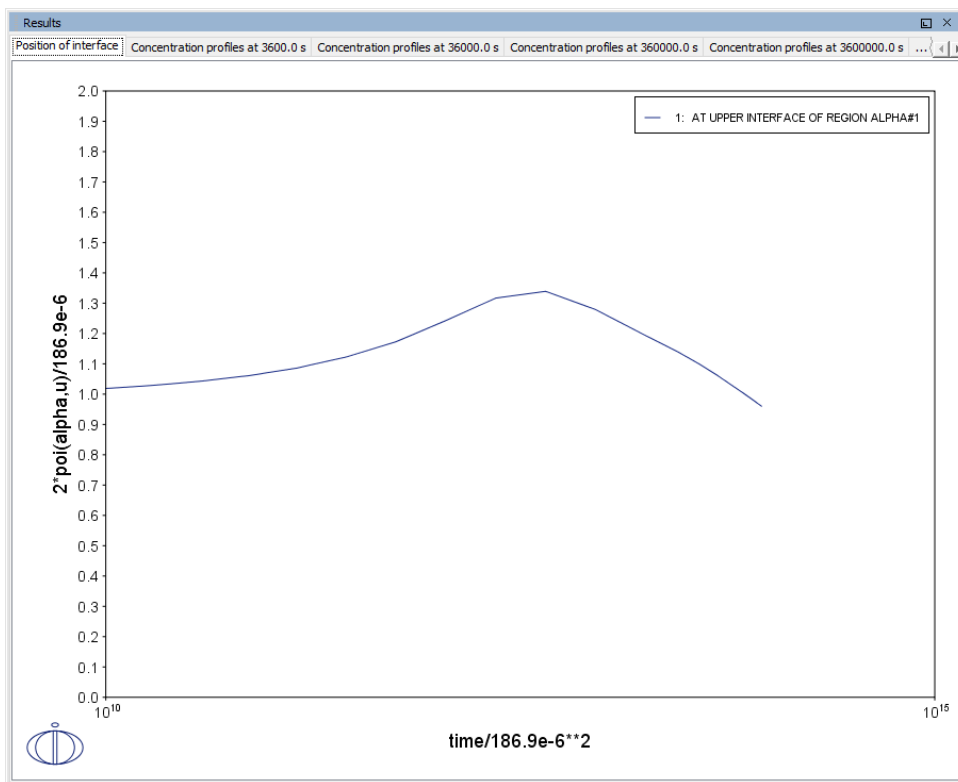
This set up corresponds to diffusion couple in Kajihara, Lim, and Kikuchi (1993)¹. Also see Kajihara and Kikuchi (1993)².



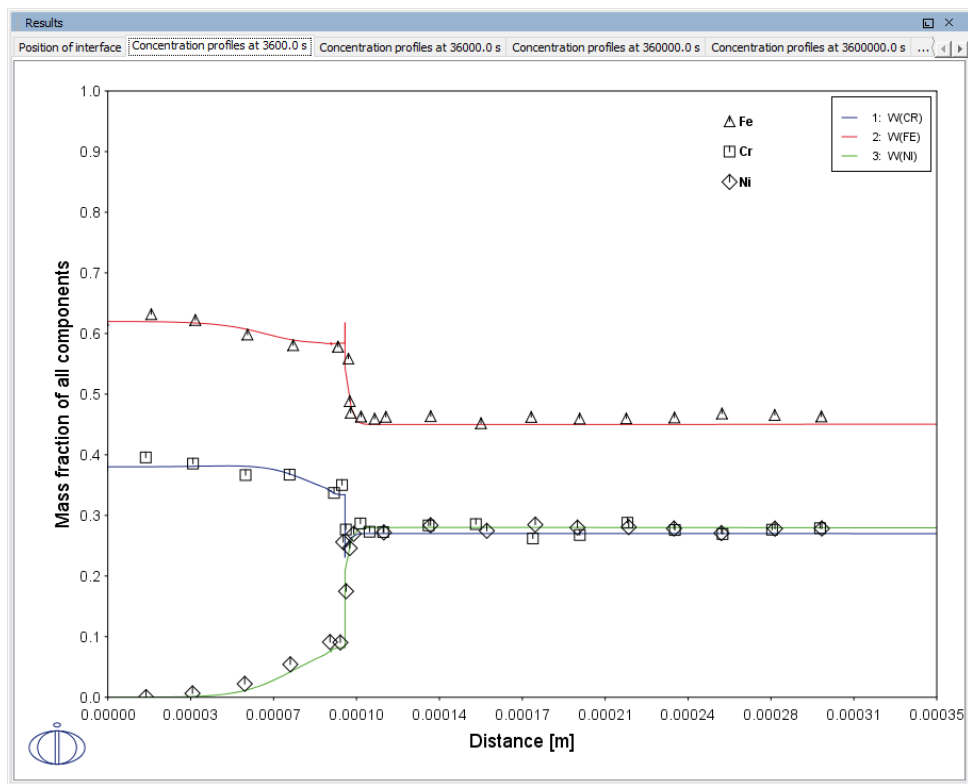
1. "Experimental Study on Dissolution of ALPHA Phase in GAMMA/ALPHA/GAMMA Diffusion Couples of the Fe-Cr-Ni System", *ISIJ Int.*, 33(4), 498–507.

2. "Numerical analysis of dissolution of α phase in $\gamma/\alpha/\gamma$ diffusion couples of the Fe-Cr-Ni system", *Acta Metall. Mat.*, 41 (7), 2045–2059.

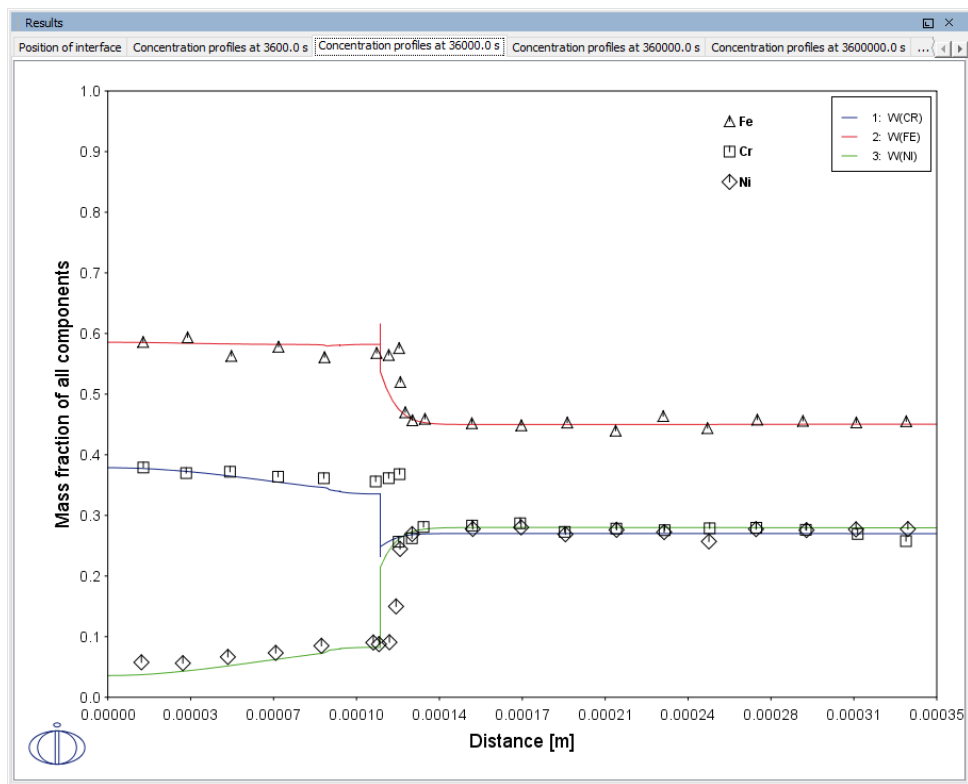
Interface Position



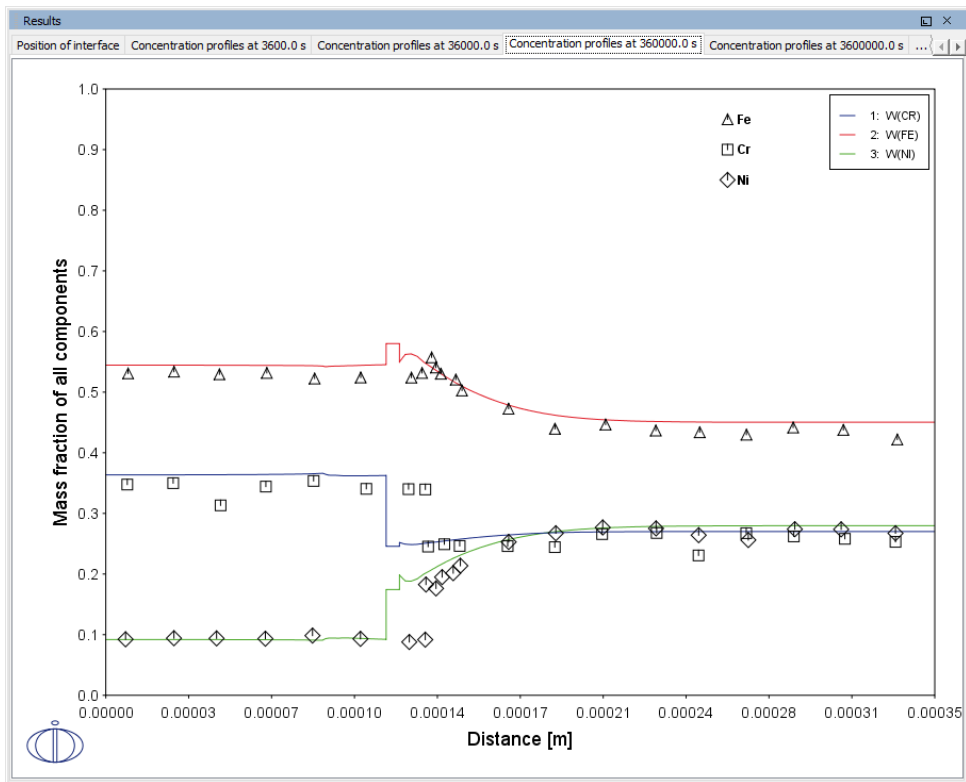
Concentration profiles at 3600 s



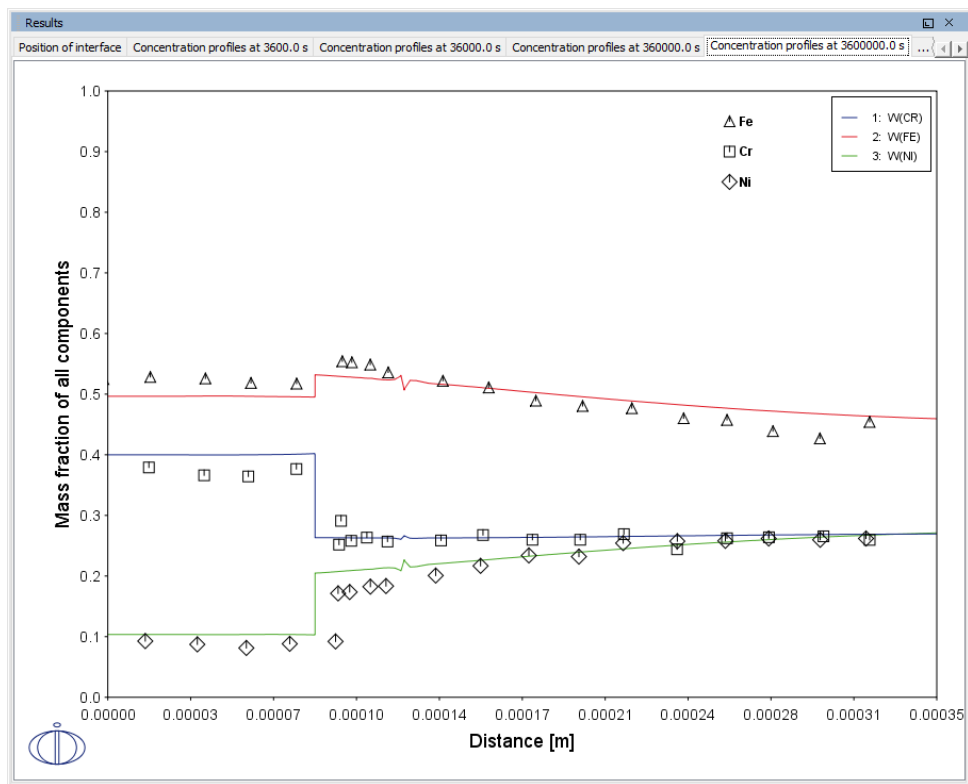
Concentration profiles at 36000 s



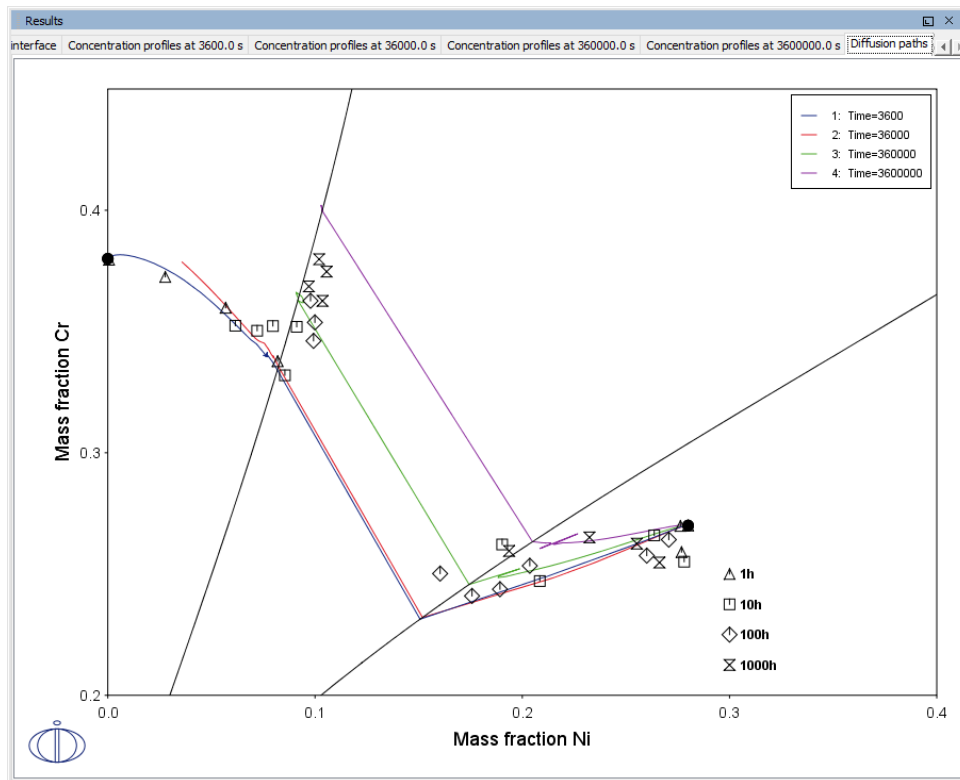
Concentration profiles at 36 0000 s



Concentration profiles at 3 600 000 s



Diffusion paths



PROJECT FILE NAME

- Folder: Diffusion Module - DICTRA
- File name: *D_05_Diffusion_Fe_Ni_Cr_Moving_Boundary_Diffusion_Couple.tcu*

D_06 Diffusion Through a Tube Wall

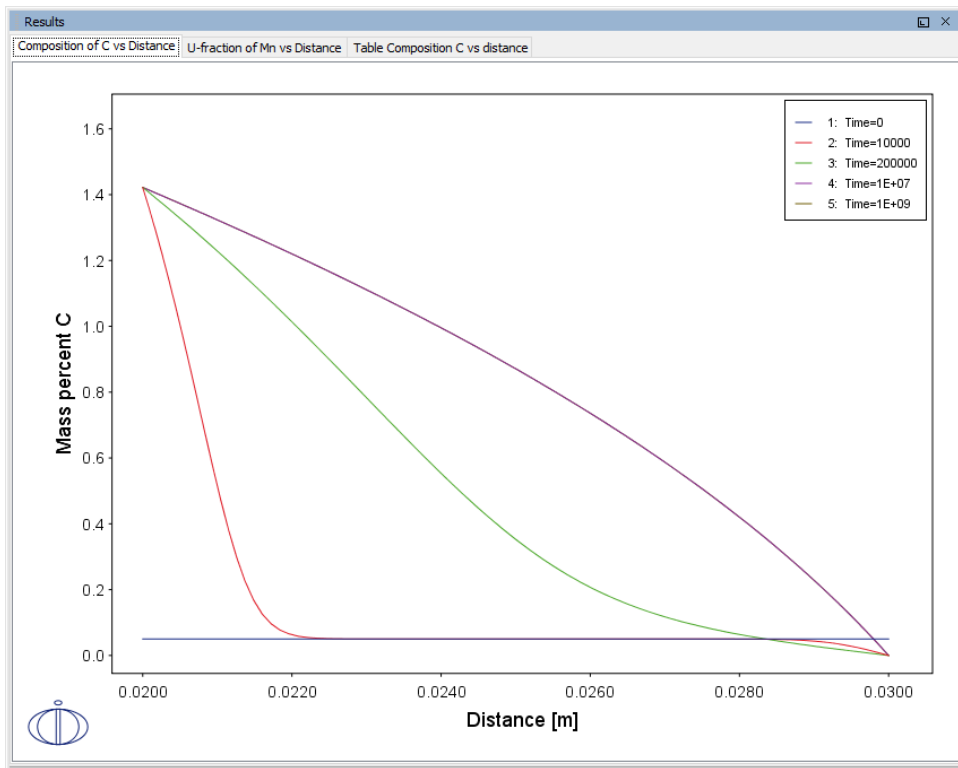
This is a simple example of diffusion through a tube wall. The tube material is an Fe-0.06Mn-0.05C alloy. Two plots comparing distance to the U-fraction of manganese and composition of carbon are generated to visualize the austenite region. A *cylindrical* geometry is used with *mixed zero flux and activity* boundary conditions.

On the inside wall a carbon activity of 0.9 is maintained whereas on the outside the carbon activity is very low. This example demonstrates the use of boundary conditions, advanced plotting and tables.



This example is based on Console Mode exab6. When in Console Mode, you can open the example from Thermo-Calc (**File** → **Examples Files** → **Diffusion Module**).

Composition of C vs Distance



U-fraction of Mn vs Distance

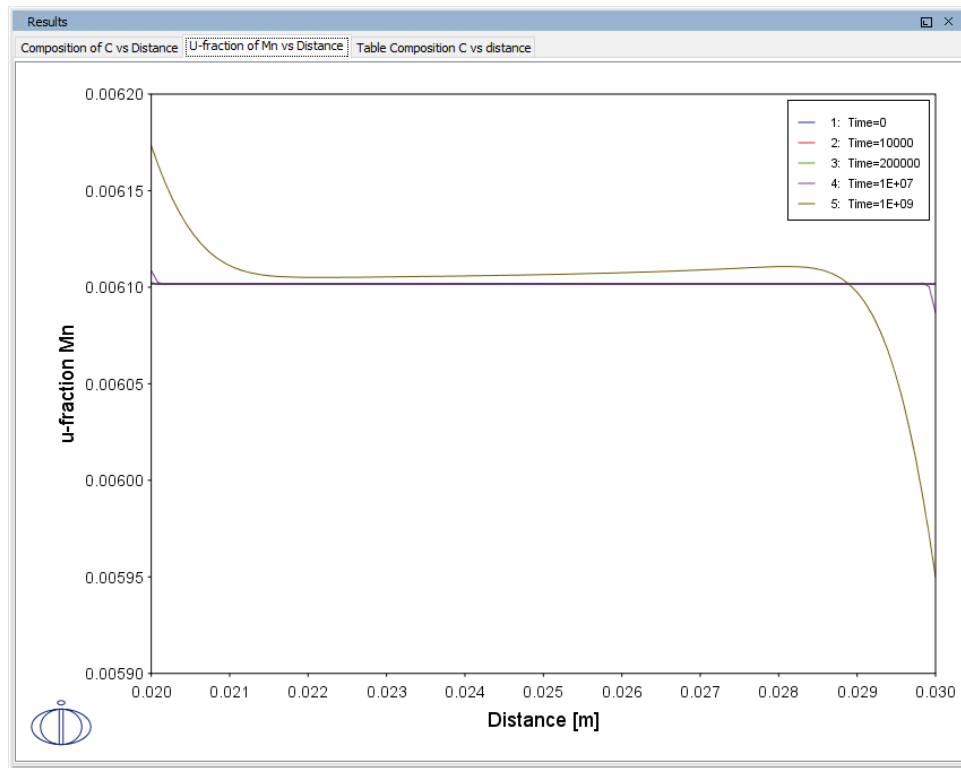
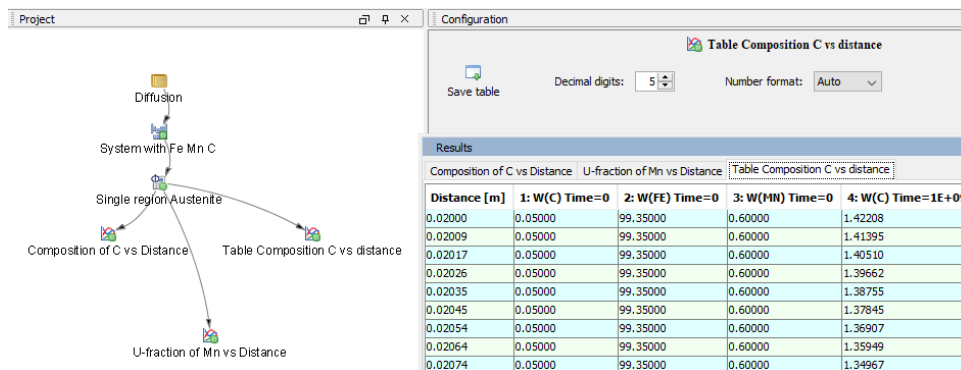


Table Composition C vs Distance



PROJECT FILE NAME

- Folder: Diffusion Module - DICTRA
- File name: *D_06_Diffusion_Carburization_Tube.tcu*

D_07 Multiphase Carburization of a Ni-25Cr-0.0001C alloy

This example is about carburization of a Ni-25Cr-0.0001C alloy. In this case the M7C3 and M3C2 carbides are entered as spheroid phases in an FCC_A1 matrix. It is similar to Graphical Mode example D_06 except the default **Simulation condition** is automatically set to use the **Homogenization** model.

The Isothermal calculation is run for 1000 hours at a temperature of 1123 K using the **Mixed zero flux and activity** left boundary condition. Results are plotted using two Plot Renderers and a Table Renderer.

This case is from Engström, Höglund, and Ågren (1994), "Computer simulation of diffusion in multiphase systems", *Met. Mat. Trans. A*, 25(6), 1127–1134.



This example is based on Console Mode exd1b. When in Console Mode, you can open the example from Thermo-Calc (**File → Examples Files → Diffusion Module**).



This example is available as a video tutorial on [our website](#) and [YouTube channel](#).

Phase fraction vs distance

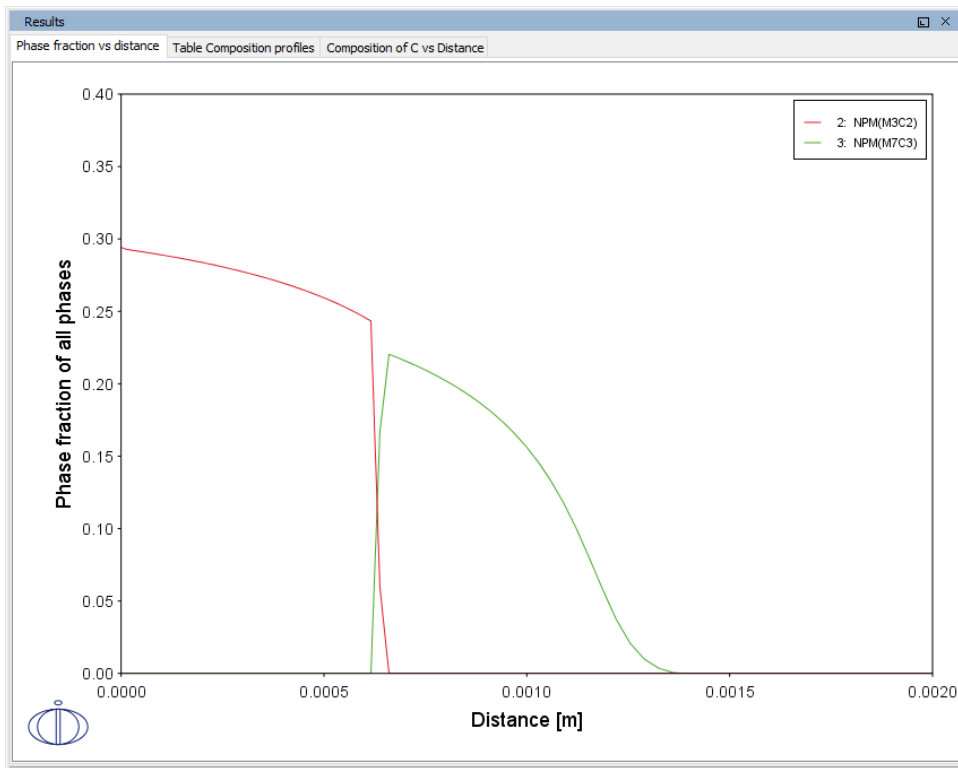
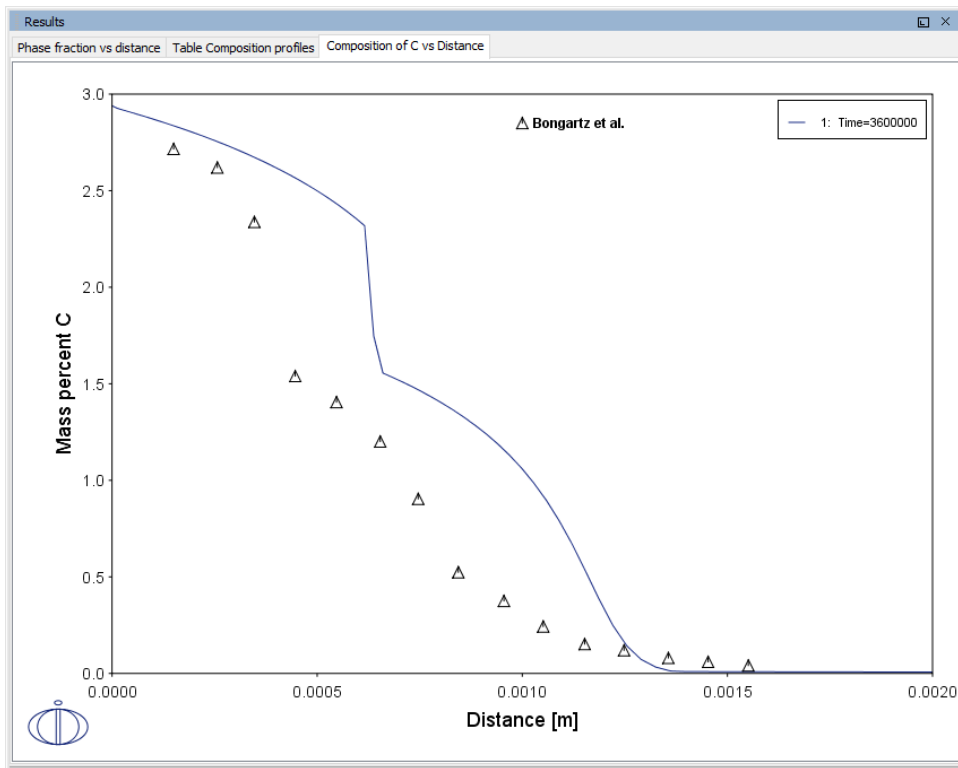


Table of Composition profiles

| Results | | | |
|----------------------------|---------|----------------------------|------------------------------|
| Phase fraction vs distance | | Table Composition profiles | Composition of C vs Distance |
| Distance [m] | 1: W(C) | 2: W(CR) | 3: W(M) |
| 0.00000 | 2.93966 | 24.35835 | 72.70199 |
| 9.88104E-6 | 2.92919 | 24.27458 | 72.79623 |
| 0.00002 | 2.92153 | 24.27324 | 72.80522 |
| 0.00003 | 2.91543 | 24.27447 | 72.81011 |
| 0.00004 | 2.90899 | 24.27584 | 72.81517 |
| 0.00005 | 2.90235 | 24.27733 | 72.82032 |
| 0.00006 | 2.89549 | 24.27886 | 72.82565 |
| 0.00007 | 2.88841 | 24.28053 | 72.83106 |
| 0.00008 | 2.88107 | 24.28222 | 72.83670 |
| 0.00010 | 2.87349 | 24.28403 | 72.84248 |
| 0.00011 | 2.86564 | 24.28588 | 72.84849 |
| 0.00012 | 2.85750 | 24.28783 | 72.85467 |
| 0.00013 | 2.84907 | 24.28984 | 72.86110 |
| 0.00014 | 2.84033 | 24.29194 | 72.86773 |
| 0.00016 | 2.83124 | 24.29412 | 72.87464 |
| 0.00017 | 2.82181 | 24.29640 | 72.88179 |
| 0.00018 | 2.81201 | 24.29877 | 72.88922 |
| 0.00020 | 2.80183 | 24.30124 | 72.89693 |
| 0.00021 | 2.79122 | 24.30381 | 72.90497 |
| 0.00022 | 2.78018 | 24.30650 | 72.91332 |
| 0.00024 | 2.76867 | 24.30930 | 72.92203 |
| 0.00025 | 2.75666 | 24.31222 | 72.93112 |
| 0.00027 | 2.74412 | 24.31528 | 72.94060 |
| 0.00028 | 2.73101 | 24.31848 | 72.95051 |
| 0.00030 | 2.71731 | 24.32182 | 72.96087 |
| 0.00031 | 2.70295 | 24.32533 | 72.97171 |
| 0.00033 | 2.68790 | 24.32901 | 72.98308 |
| 0.00035 | 2.67210 | 24.33288 | 72.99502 |
| 0.00036 | 2.65550 | 24.33694 | 73.00796 |
| 0.00038 | 2.63803 | 24.34122 | 73.02075 |
| 0.00040 | 2.61961 | 24.34573 | 73.03466 |
| 0.00042 | 2.60016 | 24.35050 | 73.04934 |
| 0.00043 | 2.57960 | 24.35554 | 73.06486 |

Composition of C vs Distance



PROJECT FILE NAME

- Folder: Diffusion Module - DICTRA
- File name: *D_07_Diffusion_Carburization_Multiphase.tcu*

Precipitation Module (TC-PRISMA) Graphical Mode Examples



Examples that use up to three elements are available to all users. The other examples require a Precipitation Module (TC-PRISMA) license to calculate and plot results.



All examples use demonstration database packages included with your installation. You can open the examples from the main menu: **File →** or **Help → Examples Files**.



Unless specified in tables for each example, all the numerical parameters are assumed default values.

P_01: Isothermal Precipitation of Al₃Sc

This example simulates the kinetics of precipitation of Al₃Sc from an FCC_A1 solution phase. The simulation results can be compared with experimental data collected from Marquis and Seidman¹ and Novotny and Ardell (2001)².

1. Marquis, E.A, and D.N Seidman. 2001. "Nanoscale Structural Evolution of Al₃Sc Precipitates in Al(Sc) Alloys." Acta Materialia 49 (11): 1909–19.

2. Novotny, Gabriel M., and Alan J. Ardell. 2001. "Precipitation of Al₃Sc in Binary Al–Sc Alloys." Materials Science & Engineering, A: Structural Materials: Properties, Microstructure and Processing 318 (1–2): 144–54.

PROJECT FILE, STEP-BY STEP INSTRUCTIONS AND VIDEO TUTORIAL INFORMATION

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_01_Precipitation_Al-Sc_AL3SC.tcu*



This example is available as a video tutorial on [our website](#) and [YouTube channel](#).



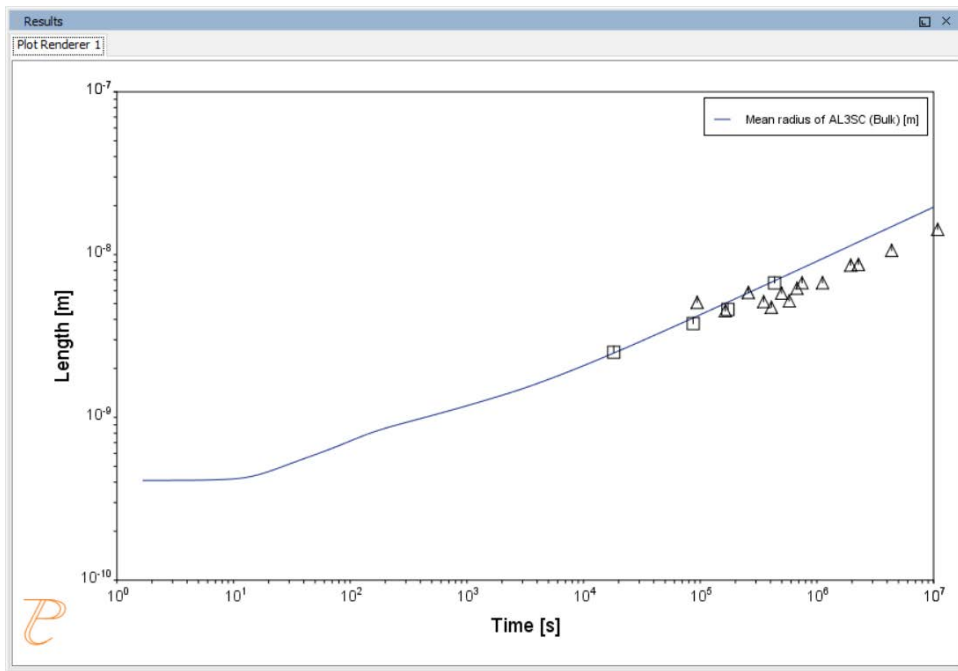
You can also use [the step-by-step instructions](#) included in a PDF to follow the video or compare to the project file in Thermo-Calc.

EXAMPLE SETTINGS

| System (System Definer) | |
|--------------------------------------------------------------|-----------------------------------------------|
| Database package | Demo: Aluminum-based alloys (ALDEMO, MALDEMO) |
| Elements | Al, Sc |
| Conditions (Precipitation Calculator) | |
| Composition | Al-0.18Sc Mole percent |
| Matrix phase | FCC_A1 |
| Precipitate phase | AL3SC |
| Precipitate Phase Data Parameters (Precipitation Calculator) | |
| Nucleation sites | Bulk |
| Interfacial energy | Calculated |
| Calculation Type (Precipitation Calculator) | |
| Calculation type | Isothermal |
| Temperature | 350° C |
| Simulation time | 1.0E7 seconds |

PLOT RESULTS

Mean radius



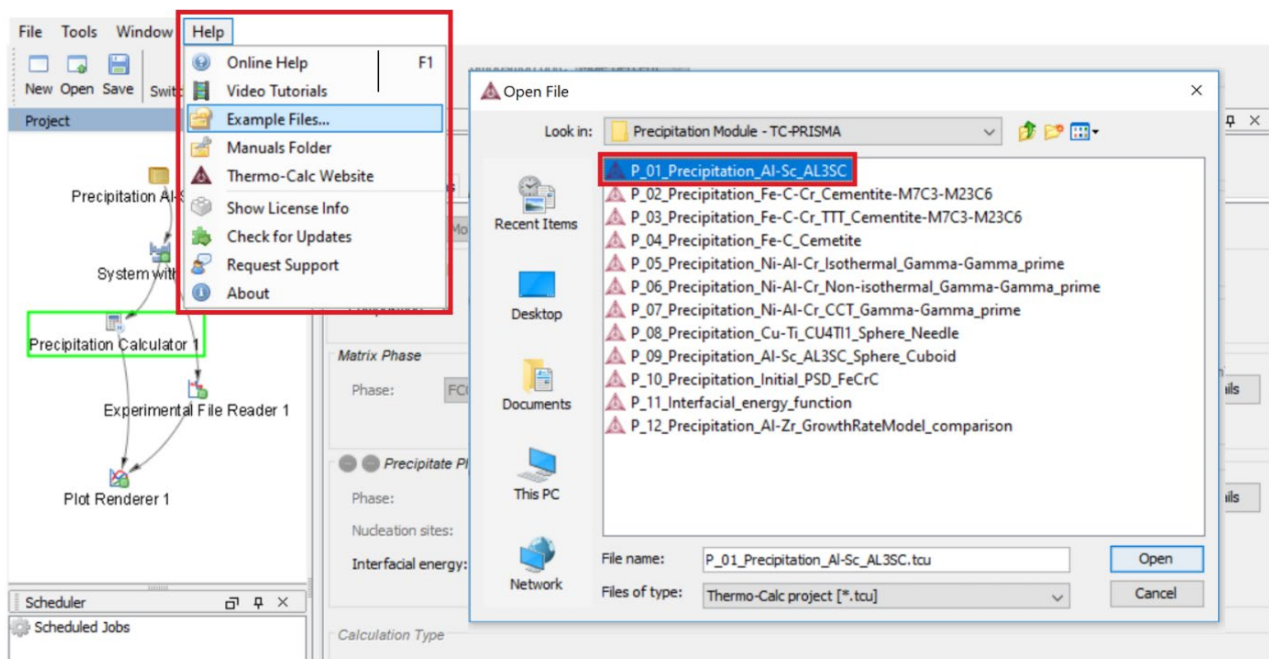
Isothermal Precipitation Calculation: Example P_01 – Precipitation Al-Sc AL3SC

This example shows you how to set up an isothermal precipitation calculation for the formation of AL3SC in an aluminium-scandium alloy at 350° using the Precipitation module (TC-PRISMA).

This is one of the most basic calculations using the Precipitation module (TC-PRISMA), so it is a good place to start if you are new to this simulation type.

HELPFUL INFORMATION

- **All users can run this calculation**, even those who do not have a license for the Precipitation module (TC-PRISMA).
- **A companion video** is available for this example , which can be watched here:
https://www.youtube.com/playlist?list=PLfv6McToaTGSpgvuLoY3b_UV-8xpgLUkj
- This calculation is based on Precipitation module example *P_01 – Precipitation Al-Sc AL3SC*, which is included in your installation. To run the example file, open Thermo-Calc and select **Help > Examples Files**. Open the *Precipitation module (TC-PRISMA)* folder. Double-click the example file and click **Perform** at the bottom centre of the **Configuration** window in Thermo-Calc.

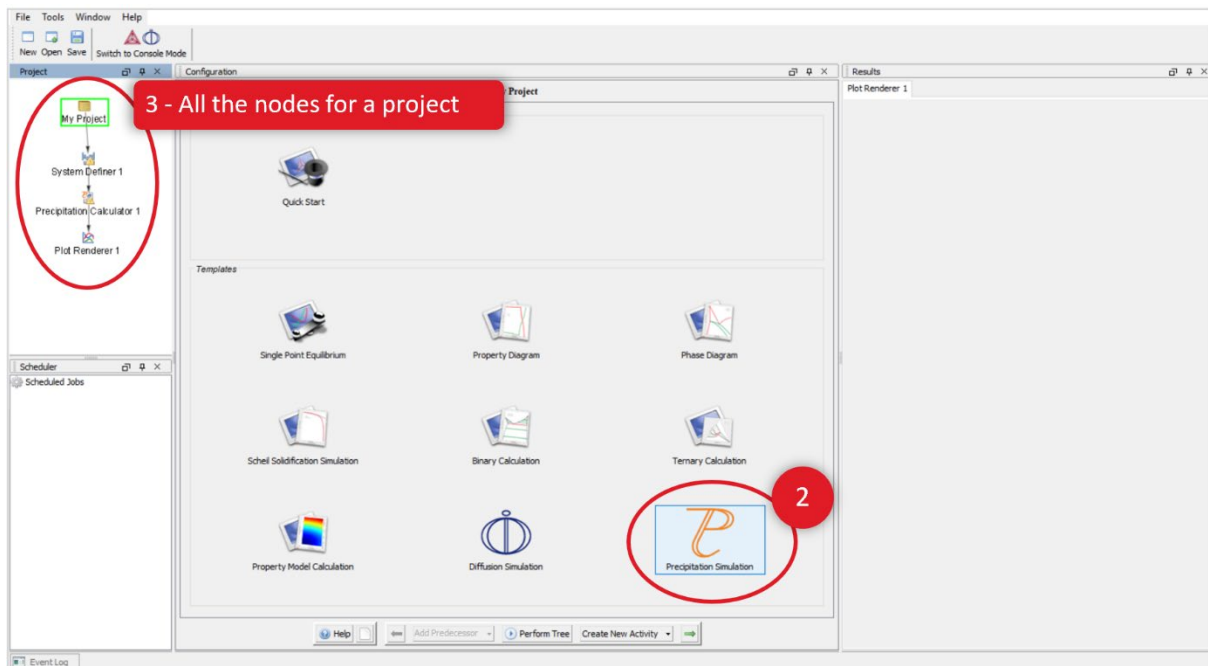


ABOUT THE EXAMPLE

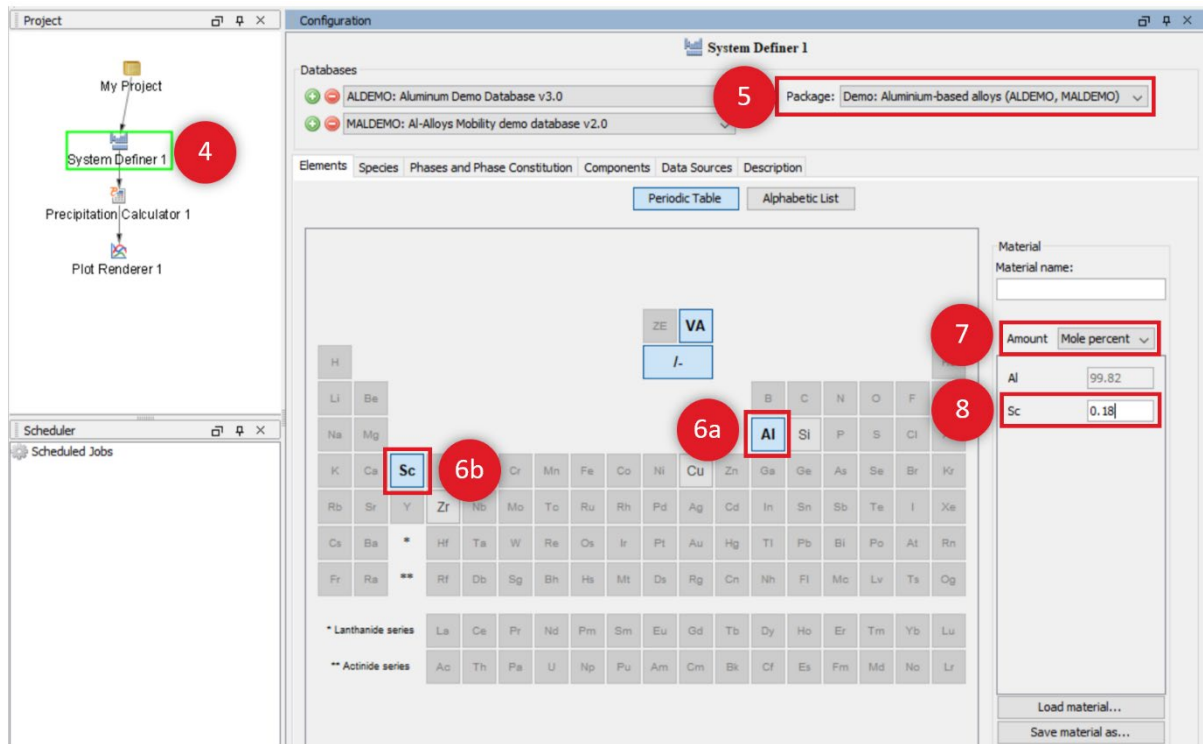
This example simulates the kinetics of precipitation of Al₃Sc from an FCC_A1 solution phase.

SETTING UP THE SYSTEM

1. Open Thermo-Calc in Graphical Mode.
2. Under templates, click **Precipitation Simulation**.
3. All the nodes for a precipitation calculation are added to the **Project** window:



4. Click the **System Definer 1** node.
5. Set the database package to **DEMO: Aluminium based alloys**, which loads both thermodynamic and kinetic demonstration aluminium databases.
6. From the periodic table, select the elements **Al** (aluminium) then **Sc** (scandium). Be sure to select Al first so that it is the dependant element.
7. Just to the right of the periodic table, select **Mole Percent** as the **Amount**.
8. Enter 0.18 for **Sc**. This automatically sets **Al** to 99.82.



Our system is now defined, but before we start the precipitation calculation, we will do a quick one axis calculation to find the phases present around 350°.

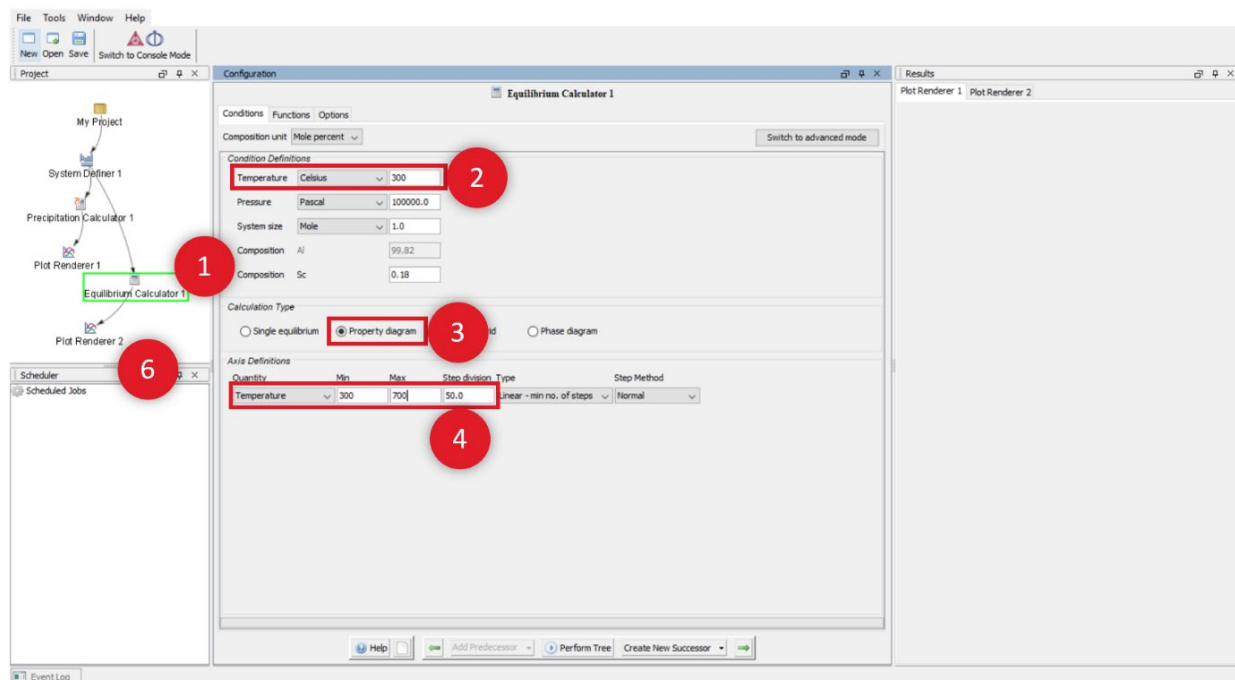
ONE AXIS CALCULATION

Why We Do This

In order to set up an isothermal precipitation calculation, we need to know which phases are present at 350°. A *one axis* calculation gives us this information.

Setting up a One Axis Calculation

1. In the **Project** window, right-click the **System Definer 1** node, and from the **Create New Successor** menu select **Equilibrium Calculator**.
2. In the **Configuration** window, select a **Temperature** in **Celsius** and enter 300.
3. Under **Calculation Type**, select **One axis**.
4. We are looking for the phases present around 350 degrees, so under **Axis Definitions** enter the **Temperature** range from **Min** 300 to **Max** 700 to capture the temperature wanted.
5. Keep the default values for everything else.
6. Our system is now defined.



7. Right-click the **Equilibrium Calculator** node and select **Create New Successor>Plot Renderer**.
8. In the **Project** window, right-click the **Plot Renderer 2** node you just created and select **Perform Now**.

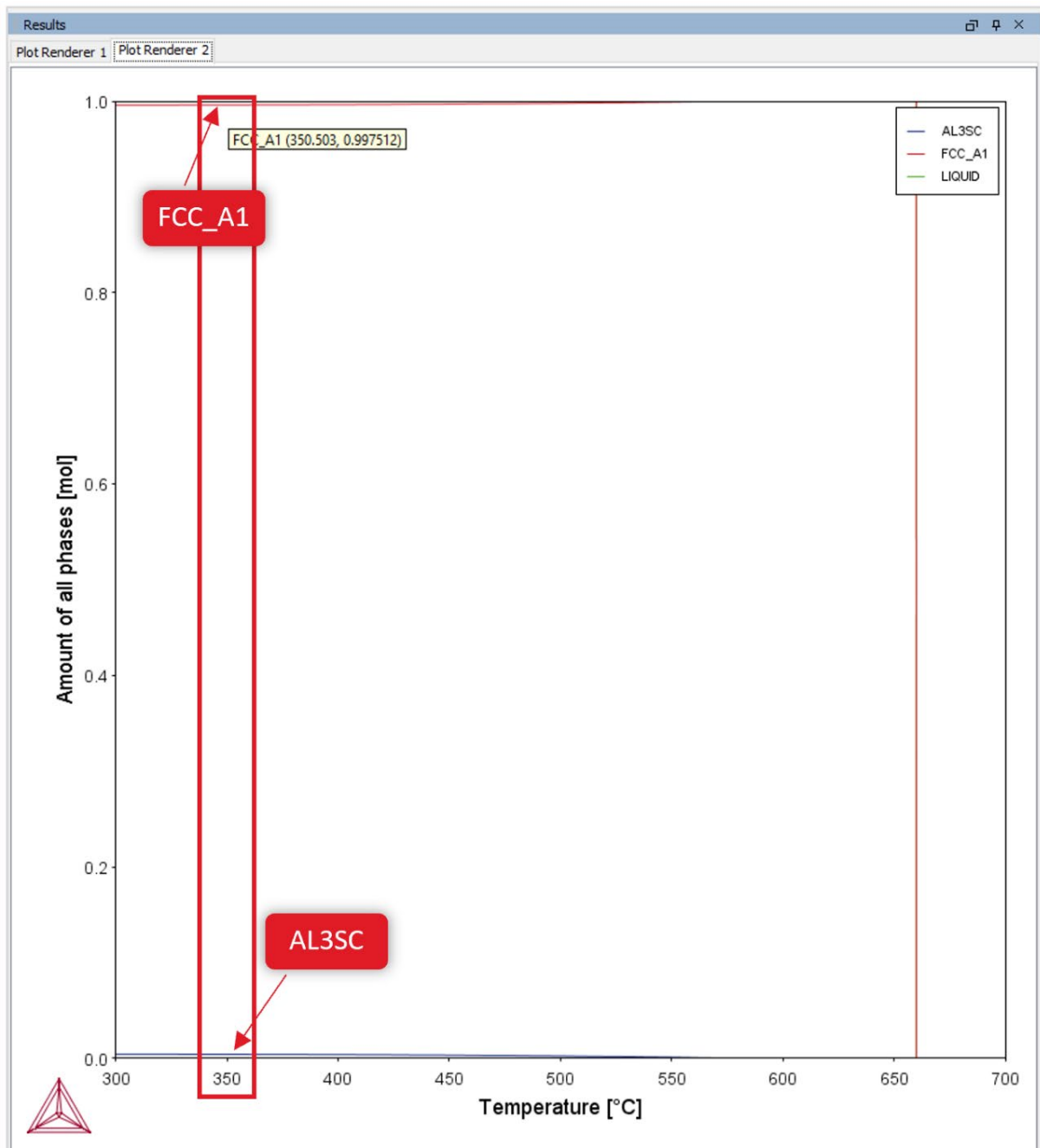
Interpreting the Results of the One Axis Calculation

Once the calculation is complete, a plot is displayed in the **Results** window. This plot shows you which phases are present at each temperature between 300° and 700° and the amount of that phase at each temperature.

If you hover your cursor over any of the lines on the plot, a label gives you the name of the phase, the temperature and the amount of the phase at that temperature.

We can see that there are two phases present at 350°. FCC_A1 is at the very top of the plot and makes up more than 99% of the system. The remainder of the system is made up of Al₃Sc, which is near the very bottom of the plot and is the precipitate phase in the alloy we are considering.

Remember these two phases because we will use them in our precipitation calculation.



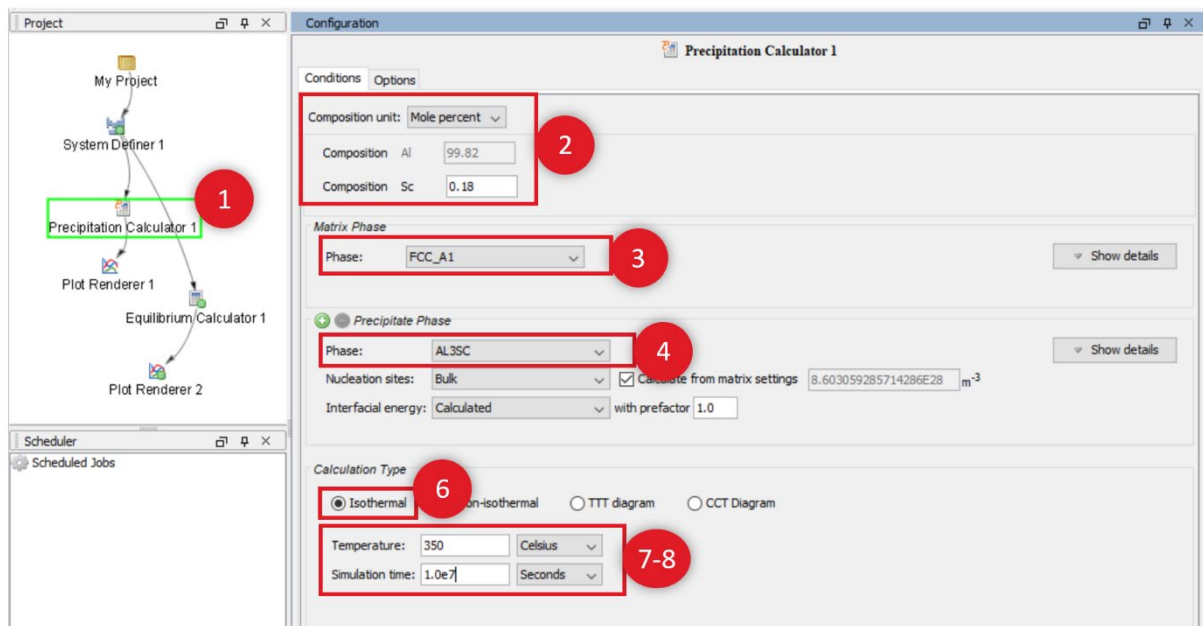
PRECIPITATION CALCULATION

Setting up the Precipitation Calculation

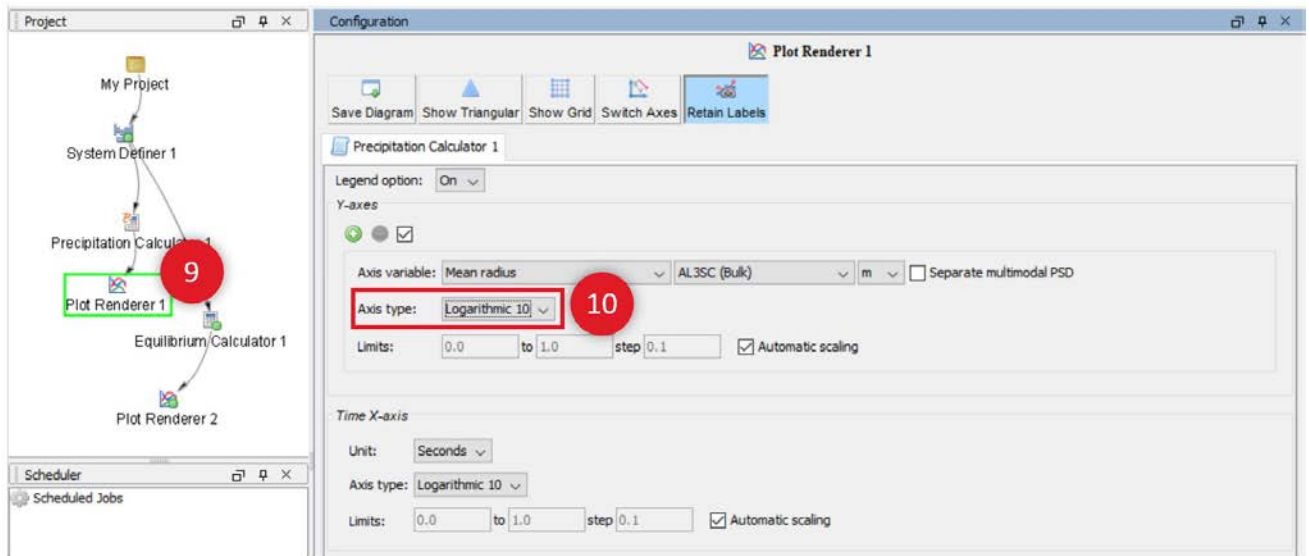
1. In the **Project** window, click the **Precipitation Calculator 1** node.
2. Notice that the composition we set in the *System Definer* auto-populated here.
3. Under *Matrix Phase*, select **FCC_A1**, which is the primary phase we saw present in the one axis calculation.

NOTE: If you do not see any phases listed here it is probably because you do not have a kinetic database selected. If so, simply go back to the *System Definer* and add a kinetic (mobility) database.

4. Under *Precipitate Phase* select **AL3SC** from the **Phase** menu because that is the other phase present around 350°, as shown in the one axis calculation.
5. Accept the default settings in the *Precipitate Phase* section. You could choose to define your own interfacial energy settings if you have them.
6. Under *Calculation Type*, make sure **Isothermal** is selected.
7. Enter 350 as the **Temperature** and select **Celsius**.
8. Enter 1.0E7 as the **Simulation time** and select **Seconds**, which is ten million seconds.

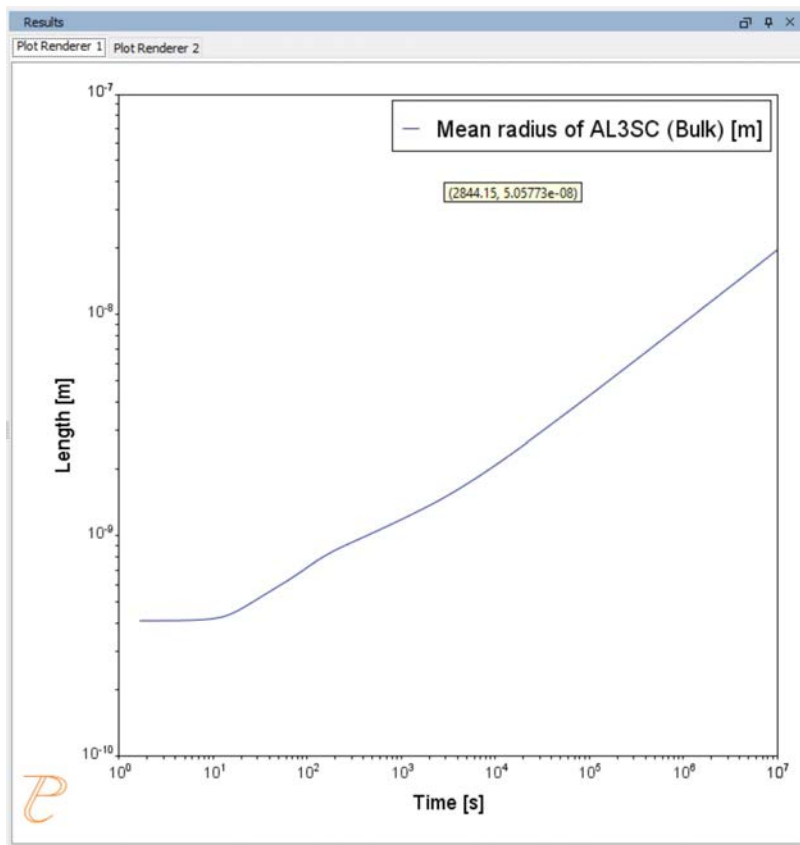


9. In the **Project** window, click the **Plot Renderer 1** node.
10. Under *Y-axes*, from the **Axis type** menu select **Logarithmic 10** for a better view of the plot.
11. Click **Perform** at the bottom, centre of the **Configuration** window.



Interpreting the Results of the Precipitation Calculation

Once the calculation is complete, your plot is shown in the **Results** window.



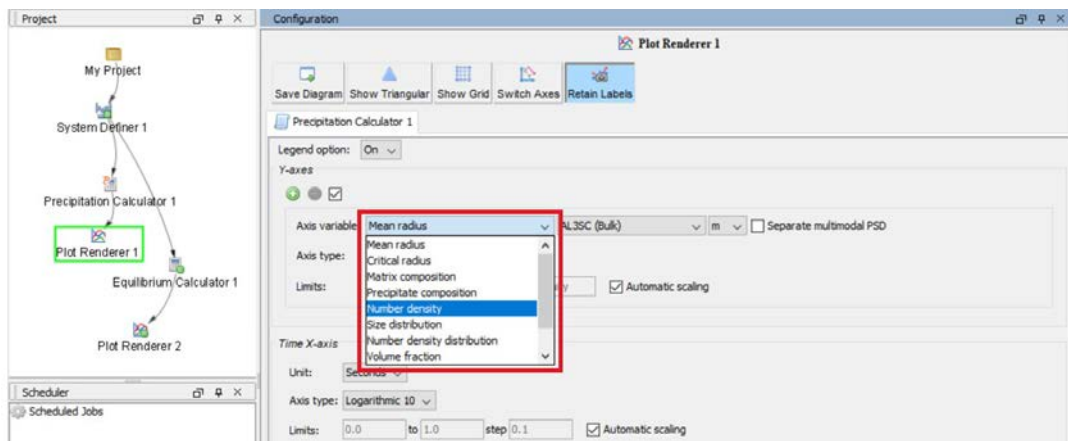
This plot shows the Mean radius of the AL3SC precipitate as a function of time.

At the beginning, which is the left-most side of the plot, the mean radius is quite small and then grows rapidly over time, which is represented by moving rightward on the plot.

Setting Other Variables in the Precipitation module (TC-PRISMA)

The Precipitation module (TC-PRISMA) offers many variables that you can plot for the same calculation.

1. Click the **Plot Renderer 1** node.
2. In the Y-axes section, select the **Axis variable** menu to see what other options are available.
3. Once you have made your selection, click **Perform** at the bottom, centre of the **Configuration** window to create a new plot.



P_02: Stable and Metastable Carbides - Isothermal

This example simulates the kinetics of precipitation of both stable and metastable carbides from ferrite phase. It demonstrates that metastable carbides (cementite, M7C3) may first emerge and then disappear and the stable phase (M23C6) prevails.

This example uses the Equilibrium Calculator and a *One axis* calculation to determine how the phases change with temperature. We are interested in the carbide precipitation at 1053K where only the carbide M23C6 is stable according to the equilibrium calculation. The Precipitation Calculator is used to do an isothermal calculation of the three phases (cementite, M23C6 and M7C3) where cementite and M7C3 are metastable phases.

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_02_Precipitation_Fe-C-Cr_Cementite-M7C3-M23C6.tcu*



Also see [our website](#) and [YouTube channel](#) for other examples of the Precipitation Module.

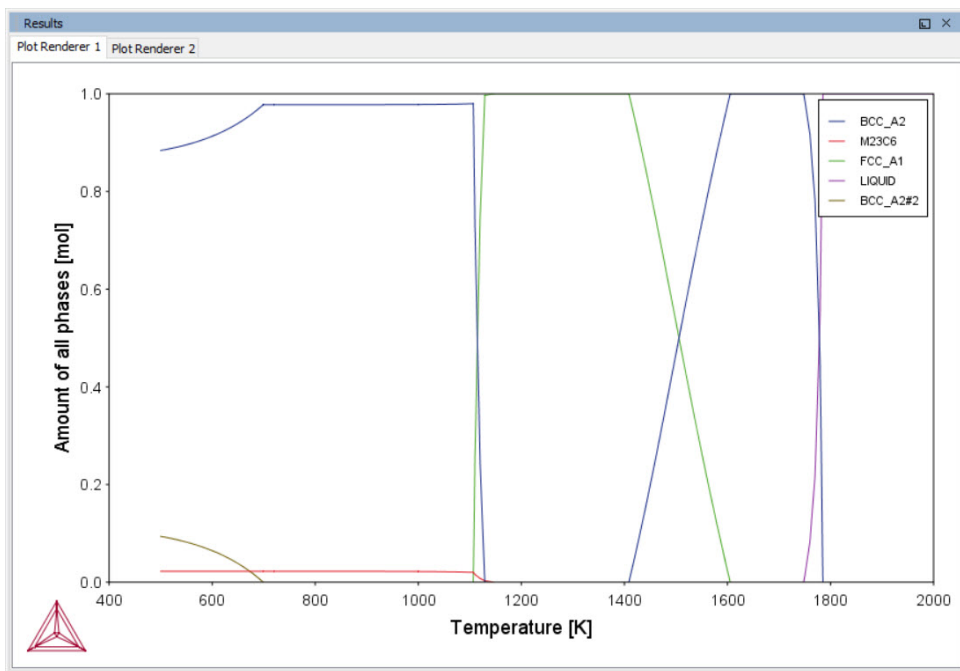
EXAMPLE SETTINGS

| System (System Definer) | |
|---------------------------------------|---------------------------------------------|
| Database package | Demo: Steels and Fe-alloys (FEDEMO,MFEDEMO) |
| Elements | Fe, C, Cr |
| Conditions (Precipitation Calculator) | |
| Composition | Fe-0.1C-12Cr Mass percent |
| Matrix phase | BCC_A2 |

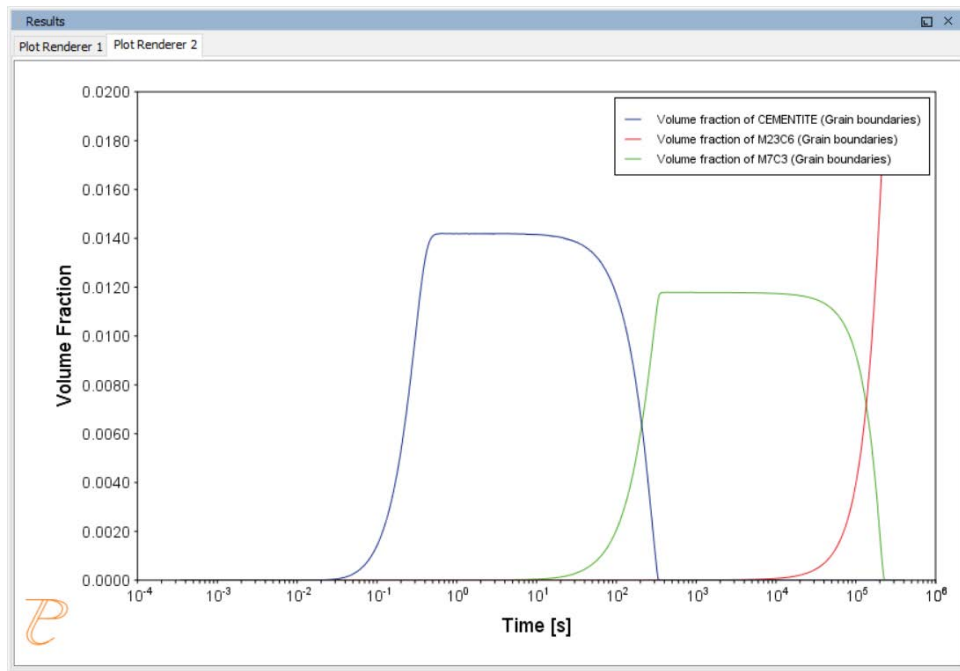
| | |
|---------------------------------------------------------------------|-----------------------------------------------------------------------------------------------|
| Precipitate phases | Cementite, M23C6 and M7C3 |
| Matrix Phase Data Parameters (Precipitation Calculator) | |
| Grain size (click Show details to display this setting) | 1.0E-4 m |
| Precipitate Phase Data Parameters (Precipitation Calculator) | |
| Nucleation sites | Grain boundaries |
| Interfacial energy | Cementite 0.167 J/m ² , M23C6 0.252 J/m ² , M7C3 0.282 J/m ² |
| Calculation Type (Precipitation Calculator) | |
| Calculation type | Isothermal |
| Temperature | 1053 K |
| Simulation time | 400 000 seconds |

PLOT RESULTS

Equilibrium Calculator: How the phases change with temperature



Precipitation Calculator: Volume fractions



P_03: Stable and Metastable Carbides - TTT Diagram

In this example, the kinetics of precipitation of both stable and metastable carbides is calculated from the ferrite phase. It demonstrates that metastable carbides may first emerge and then disappear and the stable phase prevails.

This example uses the Equilibrium Calculator and a *One axis* calculation type to determine how the phases change with temperature. Using this result, the Precipitation Calculator is used to do a TTT (Time-Temperature-Transformation) diagram calculation of the three phases (cementite, M23C6 and M7C3) at the grain boundaries.

For a TTT diagram calculation, select **TTT diagram** in **Calculation Type**, then enter **Min**, **Max**, and **Step of Temperature**, as well as **Max annealing time**. In **Stop criterion**, choose **Volume fraction of phase** and enter the value.

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_03_Precipitation_Fe-C-Cr_TTT_Cementite-M7C3-M23C6.tcu*



Also see [our website](#) and [YouTube channel](#) for other examples of the Precipitation Module.

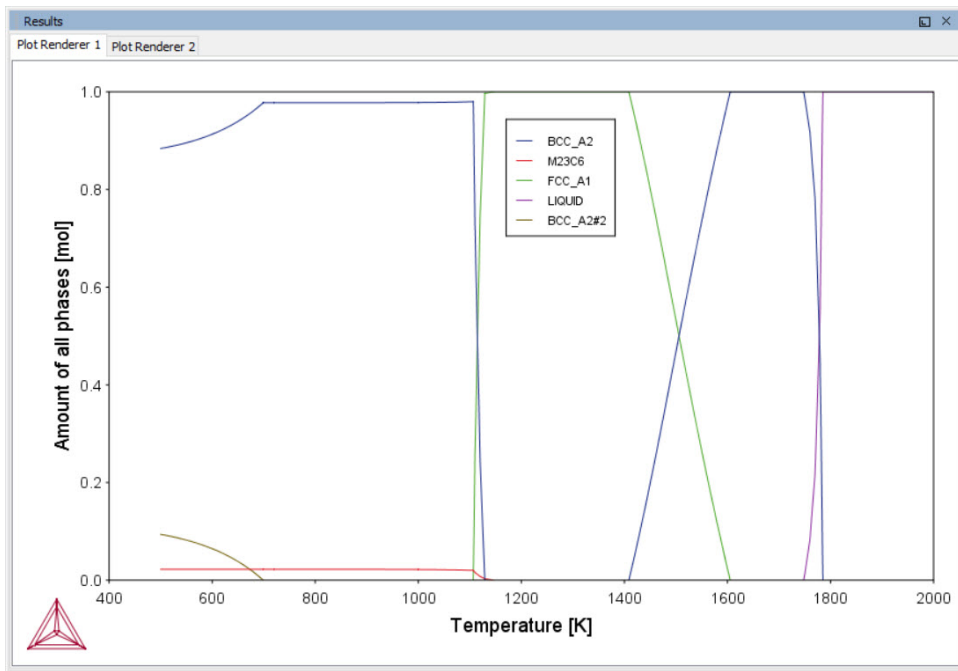
EXAMPLE SETTINGS

| System (System Definer) | |
|----------------------------------------------------------------|-----------------------------------------------------------------------------------------------|
| Database package | Demo: Steels and Fe-alloys (FEDEMO and MFEDEMO) |
| Elements | Fe, C, Cr |
| Conditions (Precipitation Calculator) | |
| Composition | Fe-0.1C-12Cr Mass percent |
| Matrix phase | BCC_A2 |
| Precipitate phases | Cementite, M23C6 and M7C3 |
| Matrix Phase Data Parameters (Precipitation Calculator) | |
| Grain size (click Show details to display this setting) | 1.0E-4 m |
| Precipitate Phase Data Parameters | |
| Nucleation sites | Grain boundaries |
| Interfacial energy | Cementite 0.167 J/m ² , M23C6 0.252 J/m ² , M7C3 0.282 J/m ² |
| Calculation Type (Precipitation Calculator) | |
| Calculation type | TTT diagram |
| Temperature | 500° to 800° C with 25° C steps |
| Max. annealing time | 1.0E8 seconds |
| Stop criteria | Volume fraction of phase is set to 0.0001 |
| Options > Numerical Parameters | |
| No. of grid points over one order of magnitude in radius | 150 |

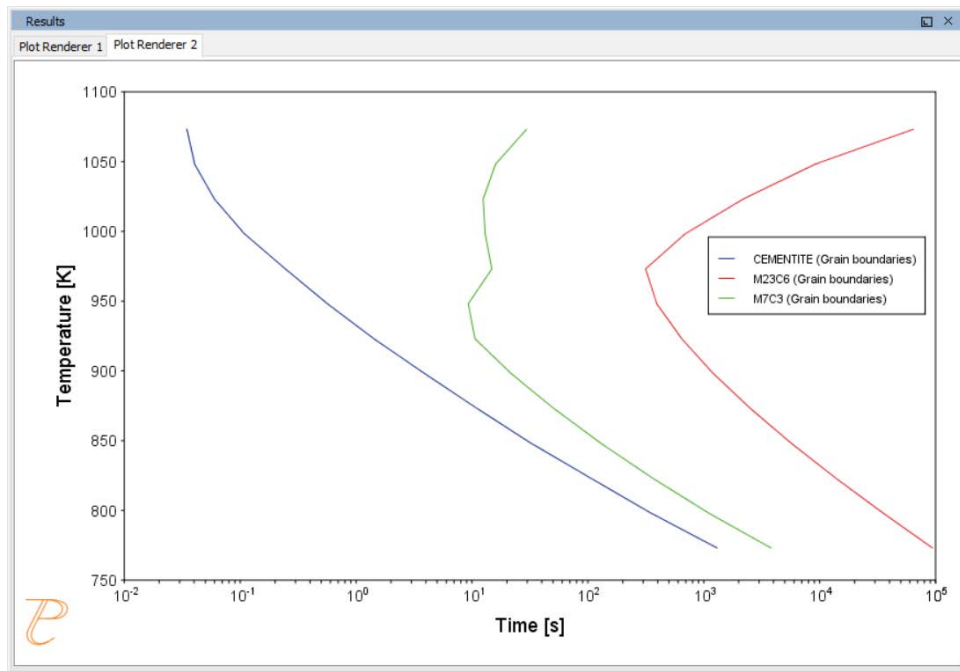
| | |
|--------------------------------------------------------------|-----|
| Max no. of grid points over one order of magnitude in radius | 200 |
| Min no. of grid points over one order of magnitude in radius | 100 |

PLOT RESULTS

Equilibrium Calculator: How the phases change with temperature



Precipitation Calculator: TTT diagram



P_04: Precipitation of Iron Carbon Cementite

Simulate the kinetics of precipitation of carbides from a BCC Fe solution phase. This example is based on Wert (1949)¹.

This example uses two Experimental File Reader activities with the Precipitation Calculator and an isothermal calculation, to plot the volume fraction of the cementite phase.

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_04_Precipitation_Fe-C_Cemetite.tcu*



Also see [our website](#) and [YouTube channel](#) for other examples of the Precipitation Module.

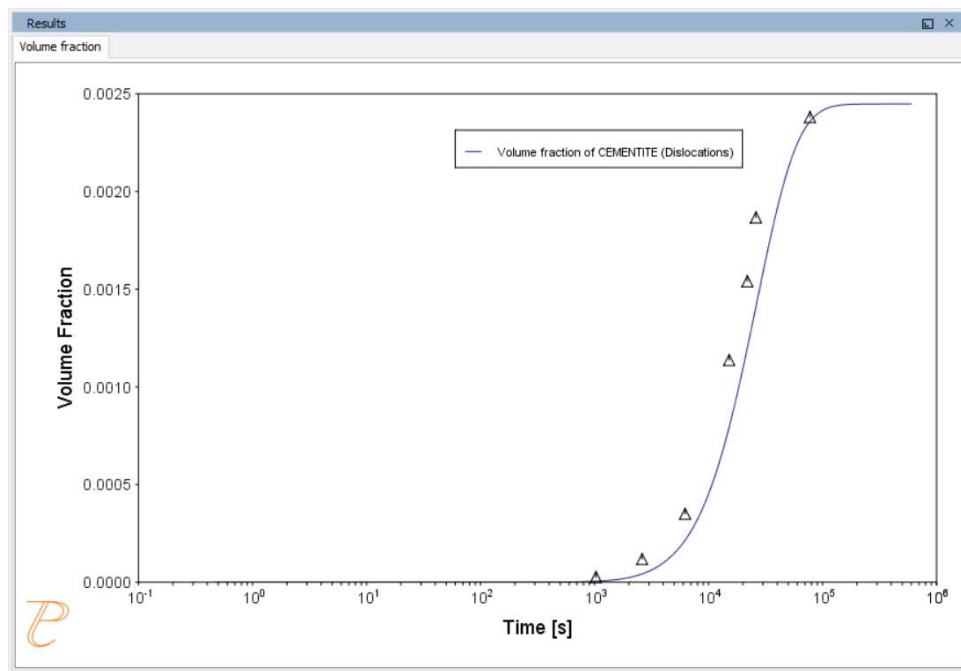
EXAMPLE SETTINGS

1. Wert, Charles A. 1949. "Precipitation from Solid Solutions of C and N in α -Iron." Journal of Applied Physics 20 (10). AIP Publishing: 943.

| System (System Definer) | |
|-------------------------------------------------------------------------|-------------------------------------------------|
| Database package | Demo: Steels and Fe-alloys (FEDEMO and MFEDEMO) |
| Elements | Fe, C |
| Conditions (Precipitation Calculator) | |
| Composition | Fe-0.016C mass percent |
| Matrix phase | BCC_A2 |
| Precipitate phase | Cementite |
| Matrix Phase Data Parameters (Precipitation Calculator) | |
| Grain aspect ratio (click Show details to display this setting) | 1.0 |
| Dislocation density (click Show details to display this setting) | 1.5e11m ⁻³ |
| Precipitate Phase Parameters (Precipitation Calculator) | |
| Nucleation sites | Dislocations |
| Interfacial energy | 0.24 J/m ² |
| Growth rate model (click Show details) | Advanced |
| Calculation Type (Precipitation Calculator) | |
| Calculation type | Isothermal |
| Temperature | 102° C |
| Simulation time | 600 000 seconds |

PLOT RESULTS

Volume Fraction



P_05: Precipitation of γ' in Ni Superalloys - Isothermal

This example simulates the kinetics of precipitation of γ' phase from γ phase. The simulation results can be compared with experimental data collected from Sudbrack et al. (2008)¹.

This example uses three Experimental File Reader activities with the Precipitation Calculator. It does an isothermal calculation to plot the volume fraction, mean radius and number density of the cementite phase.



DIS_FCC_A1 needs to be selected on the System Definer.

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_05_Precipitation_Ni-Al-Cr_Isothermal_Gamma-Gamma_prime.tcu*

¹ Sudbrack, Chantal K., Tiffany D. Ziebell, Ronald D. Noebe, and David N. Seidman. 2008. "Effects of a Tungsten Addition on the Morphological Evolution, Spatial Correlations and Temporal Evolution of a Model Ni–Al–Cr Superalloy." *Acta Materialia* 56 (3): 448–63.



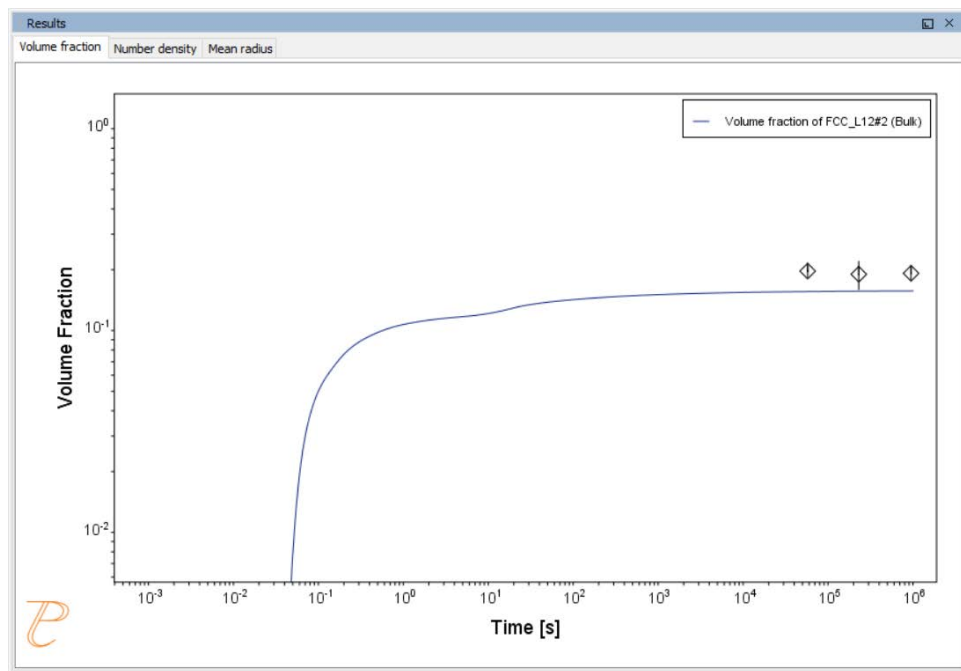
Also see [our website](#) and [YouTube channel](#) for other examples of the Precipitation Module.

EXAMPLE SETTINGS

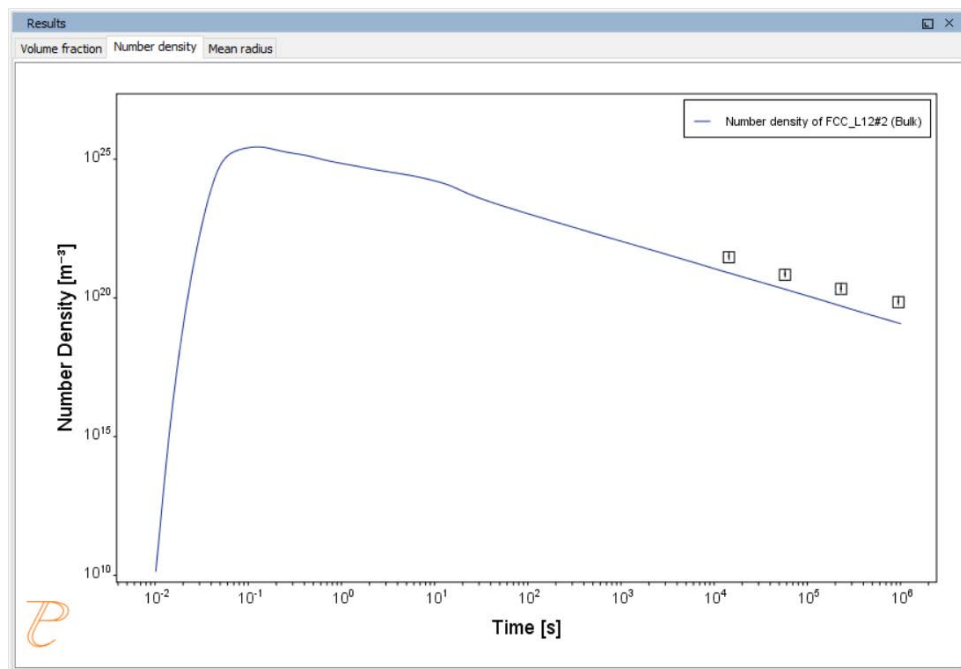
| System (System Definer) | |
|--------------------------------------------------------------|------------------------------------------------------------|
| Database package | Demo: Nickel-based Super Alloys (NIDEMO and MNIDEMO) |
| Elements | Ni, Al Cr |
| Conditions (Precipitation Calculator) | |
| Composition | Ni-9.8Al-8.3Cr Mole percent |
| Matrix phase | DIS-FCC_A1 (see note above about how to select this phase) |
| Precipitate phase | FCC_L12#2 |
| Precipitate Phase Data Parameters (Precipitation Calculator) | |
| Nucleation sites | Bulk |
| Interfacial energy | 0.012 J/m ² |
| Calculation Type (Precipitation Calculator) | |
| Calculation type | Isothermal |
| Temperature | 800° C |
| Simulation time | 1 000 000 seconds |

PLOT RESULTS

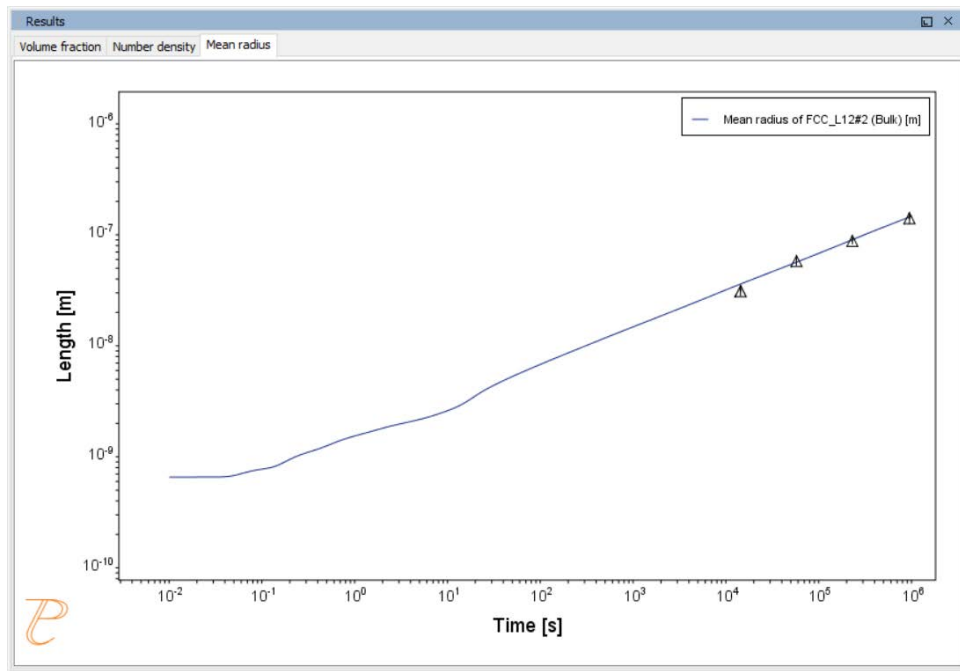
Volume Fraction



Number Density



Mean Radius



P_06: Precipitation of γ' in Ni Superalloys - Non-isothermal

This example simulates the kinetics of precipitation of γ' phase from γ phase in Ni-8Al-8Cr and Ni-10Al-10Cr at.% alloys during continuous cooling. The simulation results can be compared with experimental results from Rojhirunsakool et al. (2013)¹.



When you run (Perform) this example, it takes about 10 minutes for the calculations to complete.



DIS_FCC_A1 needs to be selected on the System Definer.

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_06_Precipitation_Ni-Al-Cr_Non-isothermal_Gamma-Gamma_prime.tcu*

¹ Rojhirunsakool, Tanaporn, S. Meher, J. Y. Hwang, S. Nag, J. Tiley, and Rajarshi Banerjee. 2013. "Influence of Composition on Monomodal versus Multimodal Γ' Precipitation in Ni-Al-Cr Alloys." *Journal of Materials Science* 48 (2): 825–31.



Also see [our website](#) and [YouTube channel](#) for other examples of the Precipitation Module.

EXAMPLE SETTINGS

In these examples a linear, continuously cooling condition is set up. This is done on the Precipitation Calculator settings window in the **Calculation Type** section:

1. Select a **Non-Isothermal**.
2. Select a **Temperature Unit** and **Time Unit** from the lists.
3. Click **Thermal Profile**, where **Time-Temperature** profile points are entered to describe the stepwise heat treatment schedule with linear segments. Up to 999 rows of data points can be entered.

In these examples two rows of data points are needed for starting time 0s and temperature 1150° C, as well as end time 3300s and temperature 380° C.

4. Click the **Plot Renderer** node to select the **Separate multimodal PSD** check box.

Plotting the size distribution from the final simulation time of 3300 seconds, you can see there are several peaks, although these are not completely separated. As above, select the **Separate multimodal PSD** check box to separate the peaks.

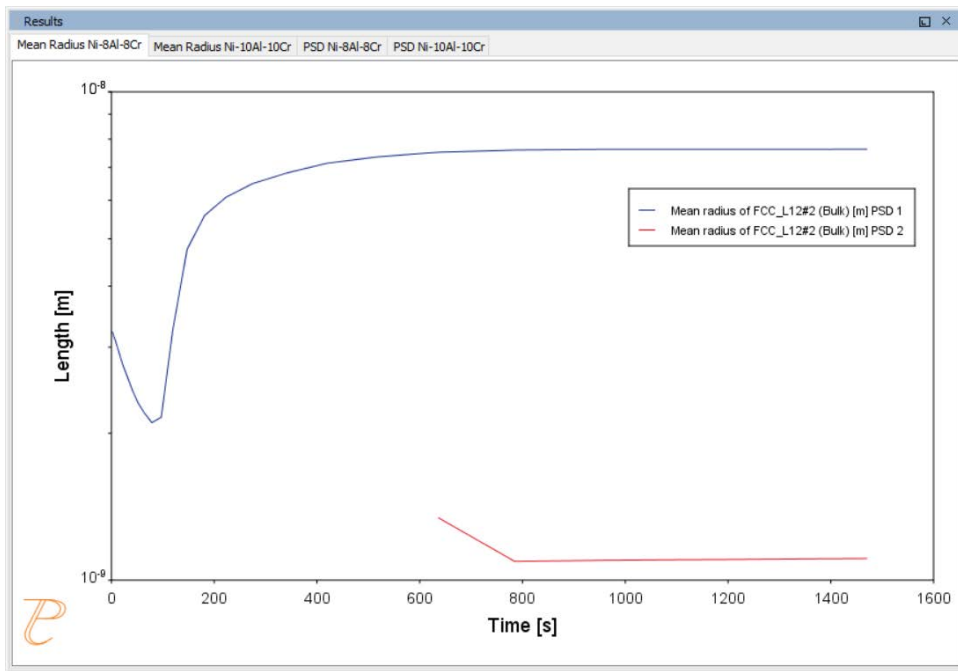
5. Adjust the **Valley depth ratio** setting to 0.05 to separate into two peaks as shown in the [Ni-10Al-10Cr plot example](#). You can experiment with this setting to see how the size distribution evolves with time, for example, try entering several values as plot times **400 600 3300**.

| System (System Definer) | |
|---------------------------------------|------------------------------------------------------------|
| Database package | Demo: Nickel-based Super Alloys (NIDEMO and MNIDEMO) |
| Elements | Ni, Al, Cr |
| Conditions (Precipitation Calculator) | |
| Composition (Ni-8Al-8Cr) | Ni-8Al-8Cr Mole percent |
| Composition (Ni-10Al-10Cr) | Ni-10Al-10Cr Mole percent |
| Matrix phase | DIS_FCC_A1 (see note above about how to select this phase) |

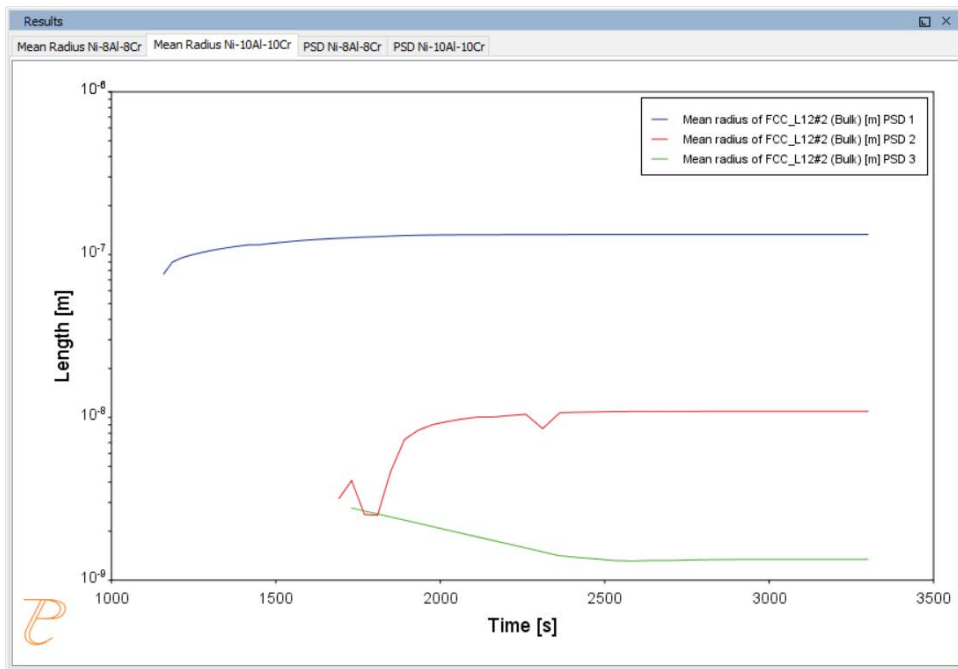
| Precipitate phase | FCC_L12#2 | | | | | | |
|------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------|------------------|-----|--------|--------|-------|
| Matrix Phase Data Parameters (Precipitation Calculator) | | | | | | | |
| Mobility enhancement prefactor (click Show details to display this setting) | 5.0 | | | | | | |
| Precipitate Phase Data Parameters (Precipitation Calculator) | | | | | | | |
| Nucleation sites | Bulk | | | | | | |
| Interfacial energy | 0.023 J/m ² | | | | | | |
| Calculation Type (Precipitation Calculator) | | | | | | | |
| Calculation type | Non-isothermal | | | | | | |
| Temperature unit | Celsius | | | | | | |
| Time unit | Seconds | | | | | | |
| Temperature | 1150 - 380 °C Edit Thermal Profile <div> <input type="button" value="Import..."/> <table border="1"> <thead> <tr> <th>Time [s]</th> <th>Temperature [°C]</th> </tr> </thead> <tbody> <tr> <td>0.0</td> <td>1150.0</td> </tr> <tr> <td>3300.0</td> <td>380.0</td> </tr> </tbody> </table> </div> | Time [s] | Temperature [°C] | 0.0 | 1150.0 | 3300.0 | 380.0 |
| Time [s] | Temperature [°C] | | | | | | |
| 0.0 | 1150.0 | | | | | | |
| 3300.0 | 380.0 | | | | | | |
| Simulation time (Ni-8Al-8Cr) | 3300 s | | | | | | |
| Simulation time (Ni-10Al-10Cr) | 3300 s | | | | | | |
| Multimodal PSD (Plot Renderer) | | | | | | | |
| Separate multimodal PSD for 8Al-8Cr | The Valley depth ratio is set to 0.05 for both plots. The number of Points is increased to 200 for an average radius plot. | | | | | | |
| Separate multimodal PSD for 10Al-10Cr | The Valley depth ratio is set to 0.18 for both plots. | | | | | | |

PLOT RESULTS

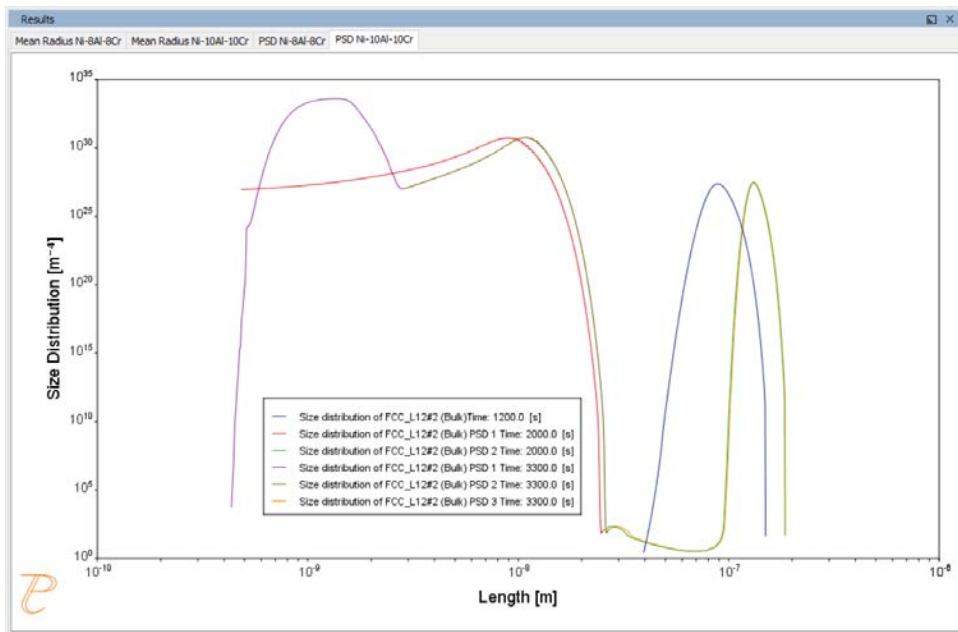
Mean Radius Ni-8Al-8Cr



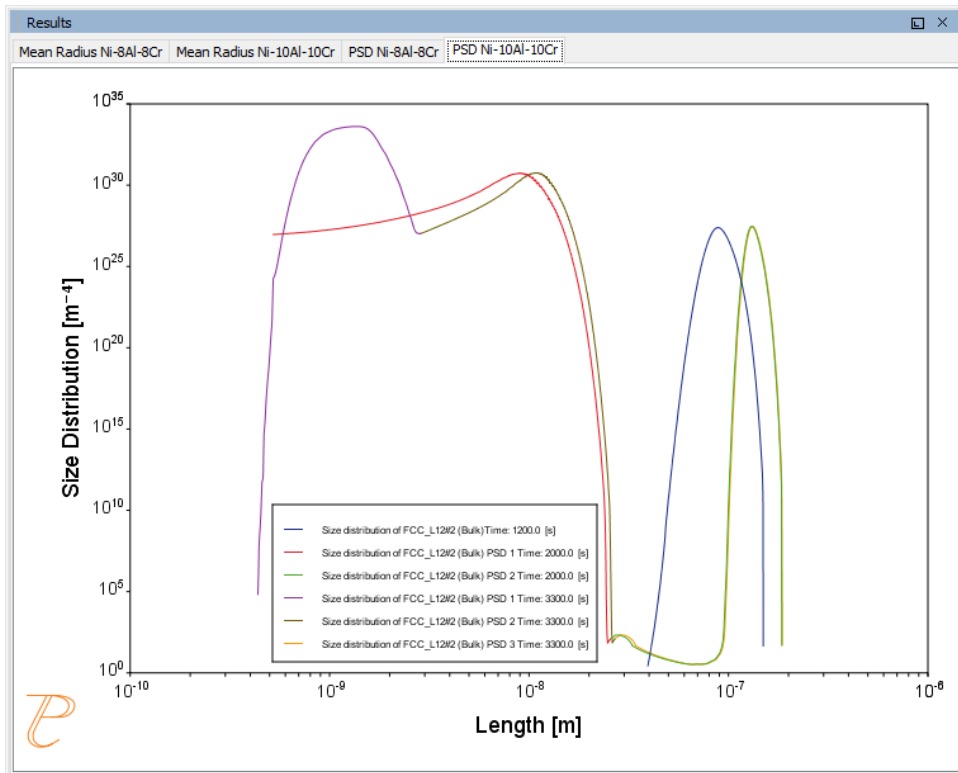
Mean Radius Ni-10Al-10Cr



Size Distribution (PSD) Ni-8Al-8Cr



Size Distribution (PSD) Ni-10Al-10Cr



P_07: Continuous Cooling Transformation (CCT) Diagram of Ni-Al-Cr γ - γ'

In this example, a Continuous Cooling Transformation (CCT) diagram for a Ni-10Al-10Cr γ - γ' alloy is calculated and plotted with superimposition of the cooling rate values.

PROJECT FILE, STEP-BY STEP INSTRUCTIONS AND VIDEO TUTORIAL INFORMATION

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_07_Precipitation_Ni-Al-Cr_CCT_Gamma-Gamma_prime.tcu*



This example is available as a video tutorial on [our website](#) and [YouTube channel](#).



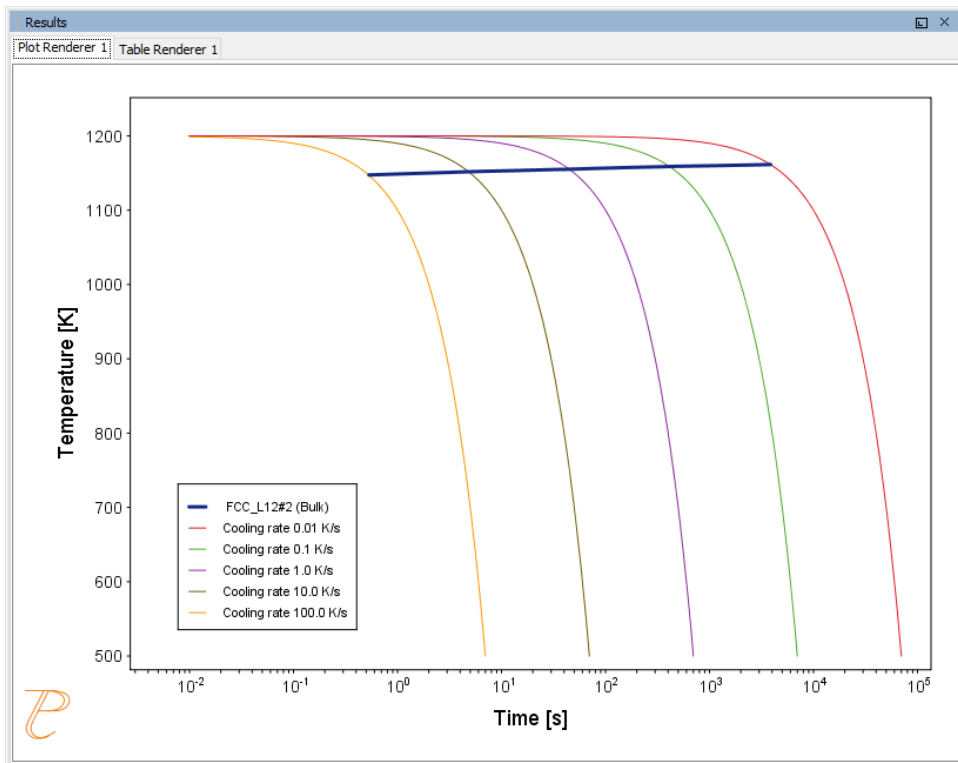
You can also use [the step-by-step instructions](#) included in a PDF to follow the video or compare to the project file in Thermo-Calc.

EXAMPLE SETTINGS

| System (System Definer) | |
|--------------------------------------------------------------|------------------------------------------------------|
| Database package | Demo: Nickel-based Super Alloys (NIDEMO and MNIDEMO) |
| Elements | Ni, Al, Cr |
| Conditions (Precipitation Calculator) | |
| Composition | Ni-10Al-10Cr Mole percent |
| Matrix phase | DIS_FCC_A1 |
| Precipitate phase | FCC_L12#2 |
| Precipitate Phase Data Parameters (Precipitation Calculator) | |
| Nucleation sites | Bulk |
| Interfacial energy | 0.023 J/m ² |
| Calculation Type (Precipitation Calculator) | |
| Calculation type | CCT Diagram |

| | |
|------------------------|---------------------------------|
| Temperature Min to Max | 500 to 1200 Kelvin |
| Cooling rate(s) | .01 .1 1 10 100 K/s |
| Stop criteria | Volume fraction of phase 1.0E-4 |

PLOT AND TABLE RESULTS

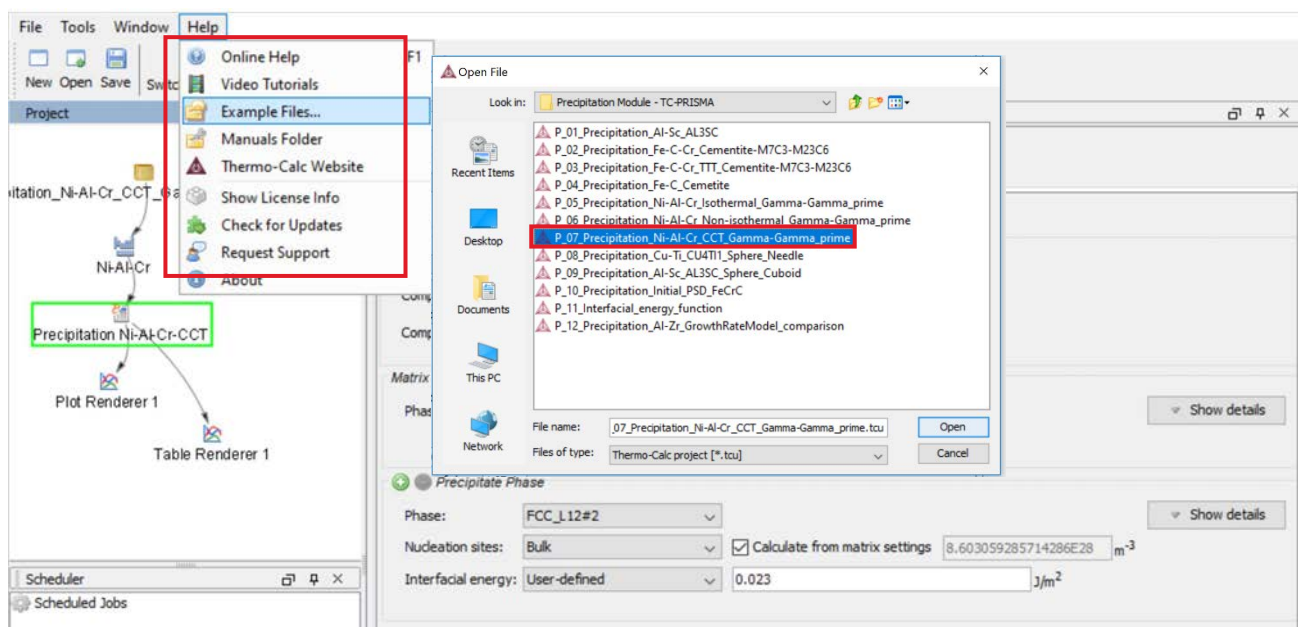


| Results | |
|-----------------|------------------|
| Plot Renderer 1 | Table Renderer 1 |
| Temperature [K] | FCC_L12#2 (Bulk) |
| 1147.52034 | 0.53291 |
| 1151.74192 | 4.83553 |
| 1155.24636 | 44.76534 |
| 1158.85368 | 411.49173 |
| 1161.48750 | 3851.47779 |

Continuous Cooling Transformation (CCT) Diagram of Ni-Al-Cr γ - γ' : Precipitation Example P_07

HELPFUL INFORMATION

- All users can run this calculation, even those who do not have a license for the Precipitation module (TC-PRISMA).
- A companion video is available for this example, which can be watched here:
https://www.youtube.com/playlist?list=PLfv6McToaTGSpqvUoY3b_UV-8xpgLUKj
- This calculation is based on Precipitation module example P_07 – *Precipitation Ni-Al-Cr CCT_Gamma-Gamma_prime*, which is included in your installation. To run the example file, open Thermo-Calc and select **Help > Examples Files**. Open the *Precipitation module (TC-PRISMA)* folder. Double-click the example file and click **Perform** at the bottom centre of the **Configuration** window in Thermo-Calc.



ABOUT THE EXAMPLE

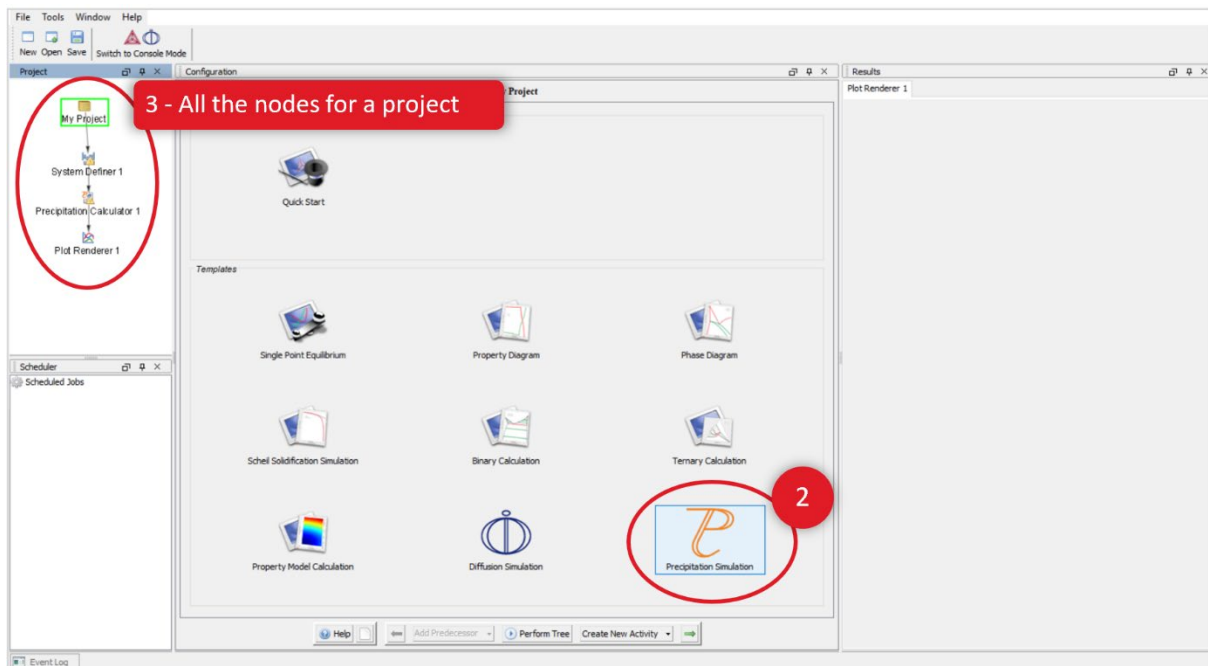
This example shows you how to simulate a CCT diagram for gamma prime (γ') precipitation in a Ni-Cr-Al alloy using the Precipitation module known as TC-PRISMA.

CCT stands for Continuous Cooling Transformation and is a calculation that maintains the same cooling rate the entire time.

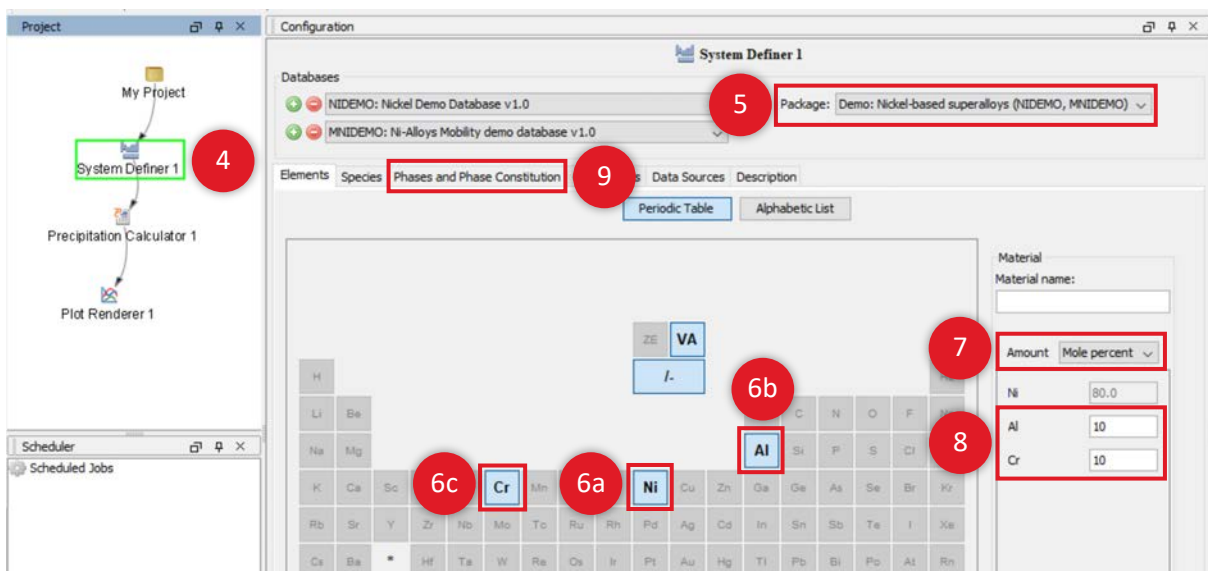
The system is a Ni-10Al-10Cr γ - γ' alloy and it is calculated and plotted with superimposition of the cooling rate values using the Precipitation module (TC-PRISMA).

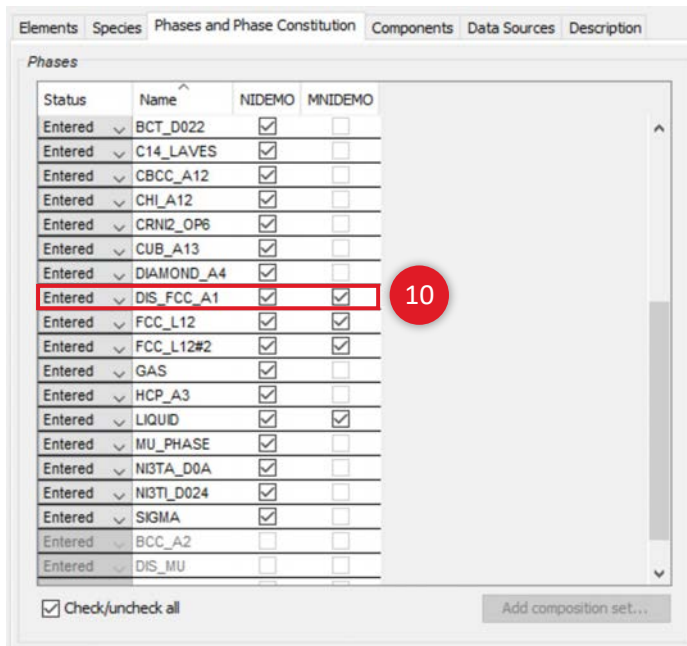
SETTING UP THE SYSTEM

1. Open Thermo-Calc in Graphical Mode.
2. Under templates, click **Precipitation Simulation**.
3. All the nodes for a precipitation calculation are added to the **Project** window:



4. Click the **System Definer 1** node.
5. Set the database package to **DEMO: Nickel based superalloys**, which loads both thermodynamic and kinetic demonstration nickel databases.
6. From the periodic table, select the elements **Ni** (nickel), **Al** (aluminium) then **Cr** (chromium). Be sure to select Ni first so that it is the dependant element.
7. Just to the right of the periodic table, select **Mole Percent** as the **Amount**.
8. Enter 10 for **Al** and 10 for **Cr**, which automatically sets **Ni** to 80 mole percent.
9. Click the **Phases and Phase Constitution** tab.



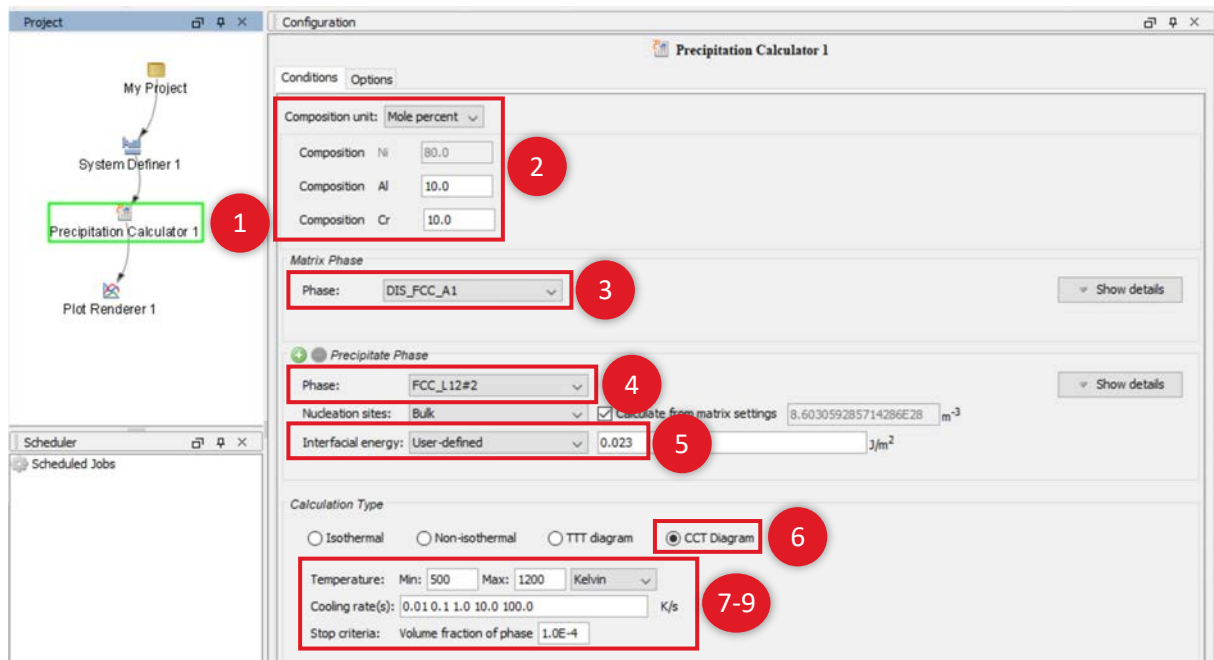


10. Click to select both check boxes next to the disordered FCC phase, **DIS_FCC_A1**.

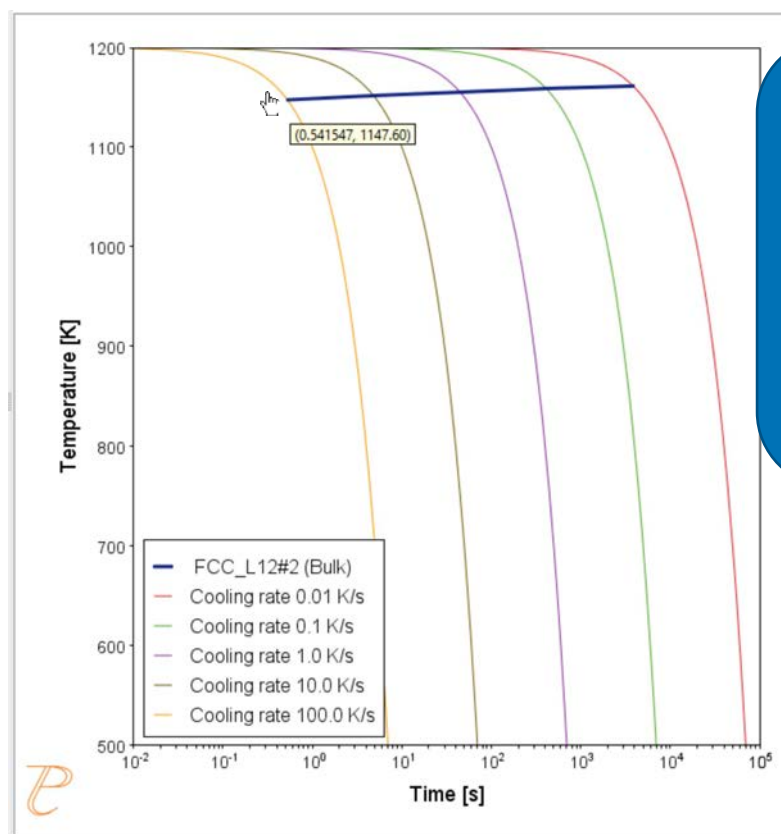
Our system is now defined, so we will set up the precipitation calculation.

SETTING UP THE PRECIPITATION CALCULATION

1. In the **Project** window, click the **Precipitation Calculator 1** node.
2. Notice that the composition we set in the **System Definer** auto-populated here.
3. Under *Matrix Phase*, from the **Phase** list select **Dis_FCC_A1**, which is the disordered FCC phase.
4. Under *Precipitate Phase* from the **Phase** list select **FCC_L12#2**.
5. Change the **Interfacial energy** to **User-defined** then enter 0.023 in the field.
6. Under *Calculation Type*, select **CCT Diagram**, which stands for Continuous-Cooling-Transformation and means that the same cooling rate is maintained throughout the calculation.
7. In the fields, set the **Min** (minimum) **Temperature** to 500 and the **Max** (maximum) to 1200 and choose **Kelvin** as the temperature unit.
8. We will enter several cooling rates for our calculation. The rates are separated by a space, so enter these values as shown: .01 .1 1 10 100.
9. Keep the default **Stop criteria** of $1E-4$ volume fraction of the γ' phase.
10. The calculation is now set, so click **Perform CCT Diagram Simulation** at the bottom, centre of the **Configuration** window.



INTERPRETING THE RESULTS OF THE PRECIPITATION CALCULATION



In this plot, the blue, horizontal line shows the time it takes for gamma prime to transform at each of the cooling rates according to the stop criteria, which we set as $1e-4$ volume fraction.

In this plot, the blue line shows the time it takes for γ' to transform at each of the cooling rates according to the stop criteria, which we set as $1e-4$ volume fraction. The cooling rates are represented by the multi-coloured curved lines.

If you hover your mouse over the intersection of the blue line and any of the vertical lines, a yellow box shows the approximate time it takes for γ' to transform according to the stop criteria, which is a volume fraction of $1e-4$, followed by the approximate temperature. In the image above, we can see a time of 0.54147 seconds and a temperature of 1147.60 Kelvin for the cooling rate of 100.0 K/s, which is represented by the yellow line.

SHOWING THE RESULTS AS A TABLE

You can also view these results in the form of a table, which gives you more precise results.

1. In the **Project** window, right-click the **Precipitation Calculator 1** node and select **Create New Successor>Table Renderer**.
2. Right-click the **Table Renderer 1** node and select **Perform Now**.

| Time [s] | FCC_L12#2 (Bulk) |
|------------|------------------|
| 0.53291 | 1147.52034 |
| 4.83553 | 1151.74192 |
| 44.76534 | 1155.24636 |
| 411.49174 | 1158.85368 |
| 3851.40881 | 1161.48822 |

Your table is shown in the **Results** window and shows the same information as in the plot - for each cooling rate the temperature and the time it takes for γ' to transform according to the stop criteria, which is a volume fraction of $1e-4$.

P_08: Precipitation of Cu-Ti CU4Ti with Assumptions of Sphere and Needle Morphologies

In this isothermal calculation example, the precipitation of Cu₄Ti phase in a Cu-Ti binary alloy is calculated. To make a comparison, two separate simulations are performed, one assuming spherical morphology without elastic strain energy, and the other assuming needle morphology whose shape, determined by competition between interfacial energy and elastic strain energy, is changed during the simulation. The transformation strain is obtained from Borchers¹. The results are compared with experiment results from Kampmann et al².



This example takes a few minutes to run.

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_08_Precipitation_Cu-Ti_CU4Ti1_Sphere_Needle.tcu*



Also see [our website](#) and [YouTube channel](#) for other examples of the Precipitation Module.

EXAMPLE SETTINGS



To ensure that the settings are done on the correct Precipitation Calculators, the **Sphere** and **Needle** nodes are renamed from **Precipitation Calculator** to match their morphology. The morphology is set in the **Precipitate Phase** section when you click **Show details**.

System (System Definer)

Database package

Demo: Copper-based alloys (CUDEMO and MCUDEMO)

1. Borchers C. 1999. "Catastrophic Nucleation during Decomposition of Cu-0.9at.%Ti." Phil. Mag. A 79(3):537-547

2. Kampmann R., Eckerlebe H., and Wagner R. 1987. "Precipitation Kinetics in Metastable Solid Solutions - Theoretical Considerations and Application to Cu-Ti Alloys." Mat. Res. Soc. Symp. Proc. 57: 525-542.

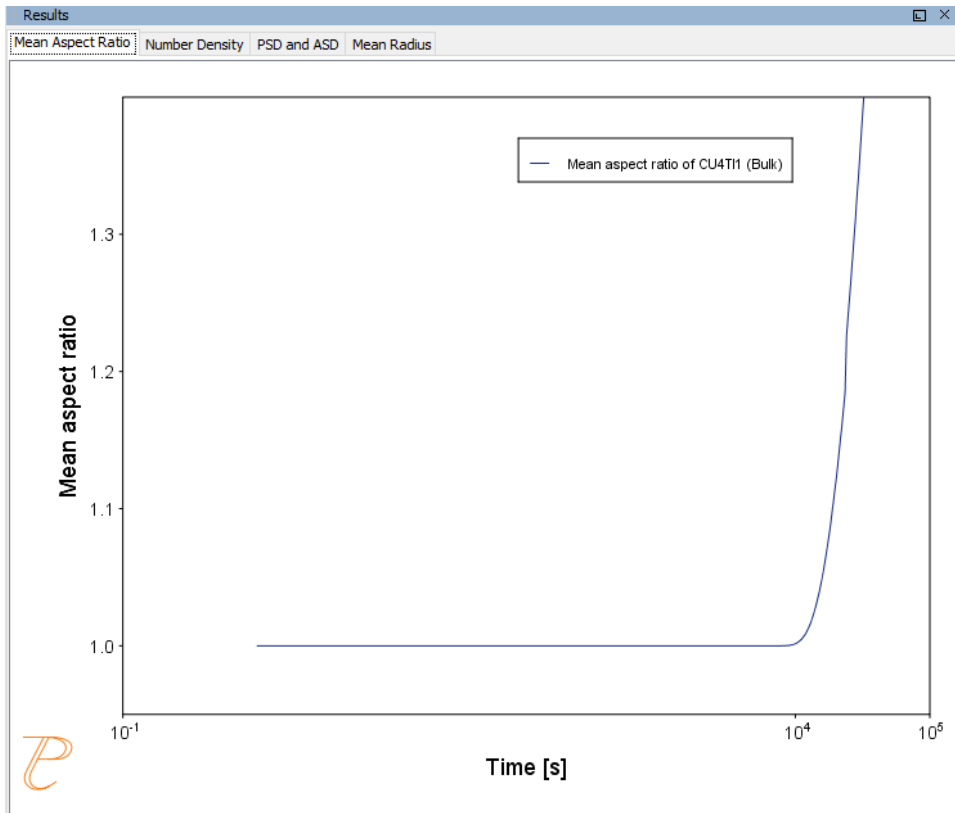
| | |
|------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Elements | Cu, Ti |
| Sphere and Needle Conditions (Precipitation Calculator) | |
| Composition | Cu-1.9Ti Mole percent |
| Matrix phase | FCC_L12 |
| Precipitate phase | CU4TI1 |
| Matrix Phase Data Parameters (Precipitation Calculator) | |
| Mobility enhancement prefactor (click Show details to display this setting) | 100 |
| Precipitate Phase Data Parameters (Precipitation Calculator) | |
| Nucleation sites | Bulk |
| Interfacial energy | The default |
| Morphology (click Show details to display this setting) | <p>For the Sphere node (renamed from Precipitation Calculator), keep the default.</p> <p>For the Needle node (renamed from Precipitation Calculator), Needle is selected.</p> |
| Transformation strain (click Show details to display this setting) | <p>For the Sphere node (renamed from Precipitation Calculator), keep the default.</p> <p>For the Needle node (renamed from Precipitation Calculator), User defined is selected. In this example, the following settings are defined:</p> <ul style="list-style-type: none"> • ϵ_{11} and ϵ_{22} are set to 0.022 • ϵ_{33} is set to 0.003 |
| Calculation Type (Precipitation Calculator) | |
| Calculation type | Isothermal |
| Temperature | 350° C |
| Simulation time | 10,000 seconds |
| Datasets (Experimental File Reader) | |
| Borchers Mean radius vs Time | Data sets included with this example and imported to two Experimental |

and Borchers Number density
vs Time

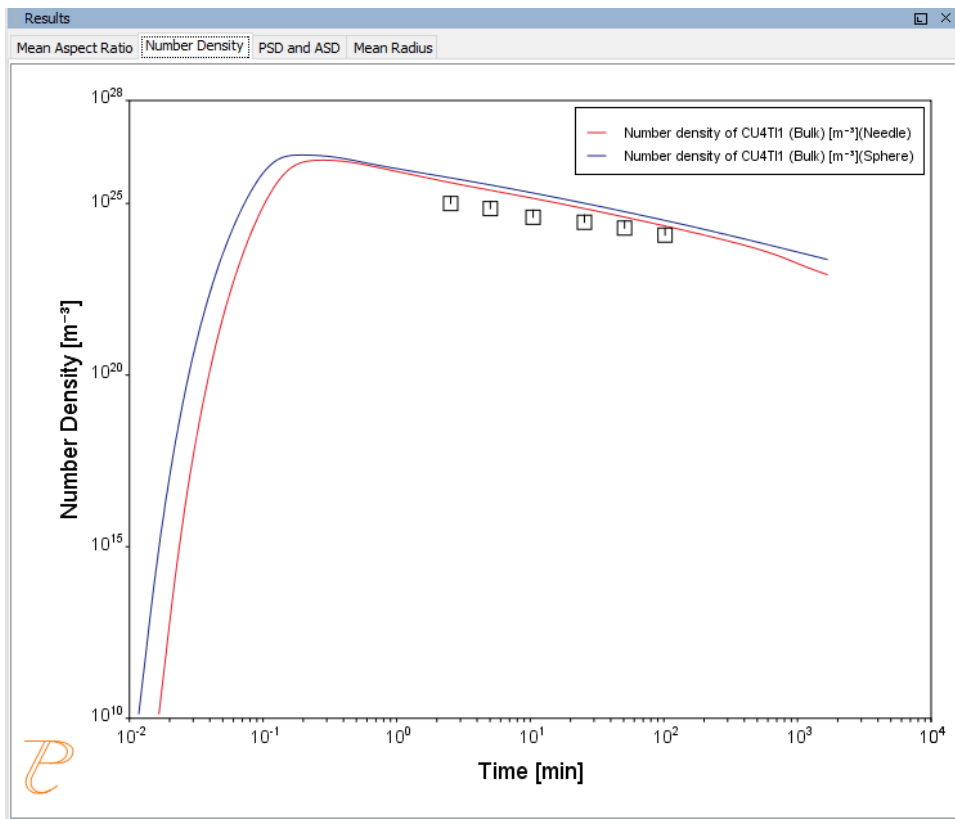
File Readers. These data sets are used for the Mean Radius and Number
Density plots, respectively.

PLOT RESULTS

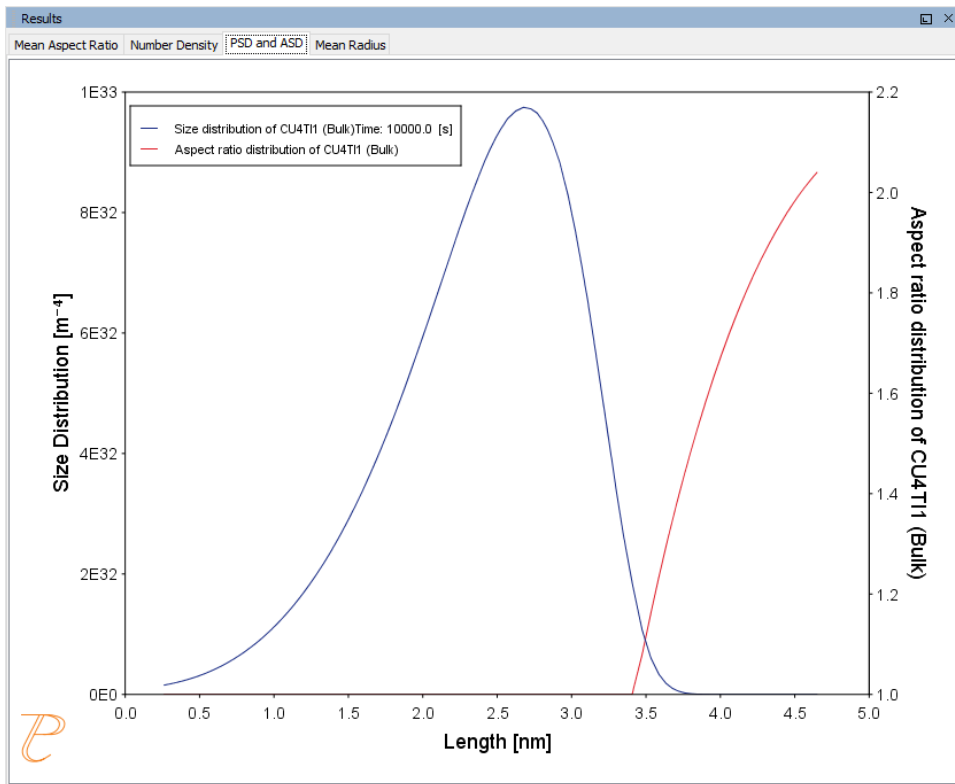
Mean Aspect Ratio



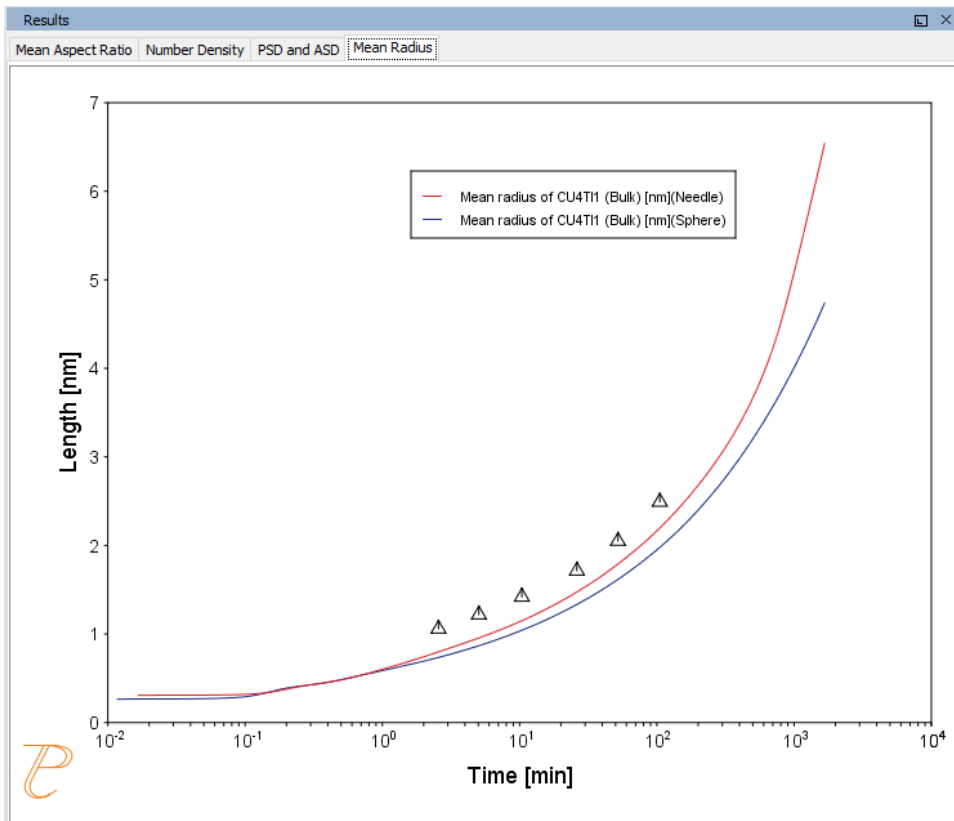
Number Density



PSD and ASD



Mean Radius



P_09: Precipitation of Al-Sc Al₃Sc with Assumption of Sphere and Cuboid Morphologies

In this isothermal calculation example, the precipitation of Al₃Sc phase from FCC_A1 matrix phase in an Al-Sc binary alloy is simulated. To make a comparison, two separate calculations are performed, one assuming spherical morphology without elastic strain energy, and the other assuming cuboid morphology whose shape is determined by competition between interfacial energy and elastic strain energy. The simulation results are compared with experimental data collected from Marquis and Seidman¹ and Novotny and Ardell (2001)². In addition, mean cubic factor and cubic factor distribution are also plotted for cuboid shape to illustrate the spherical-cuboidal transition during precipitation.

PROJECT FILE, STEP-BY STEP INSTRUCTIONS AND VIDEO TUTORIAL INFORMATION

1. Marquis, E.A, and D.N Seidman. 2001. "Nanoscale Structural Evolution of Al₃Sc Precipitates in Al(Sc) Alloys." *Acta Materialia* 49 (11): 1909–19.

2. Novotny, Gabriel M., and Alan J. Ardell. 2001. "Precipitation of Al₃Sc in Binary Al–Sc Alloys." *Materials Science & Engineering, A: Structural Materials: Properties, Microstructure and Processing* 318 (1–2): 144–54.

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_09_Precipitation_Al-Sc_AL3SC_Sphere_Cuboid.tcu*



This example is available as a video tutorial on [our website](#) and [YouTube channel](#).



You can also use [the step-by-step instructions](#) included in a PDF to follow the video or compare to the project file in Thermo-Calc.

EXAMPLE SETTINGS



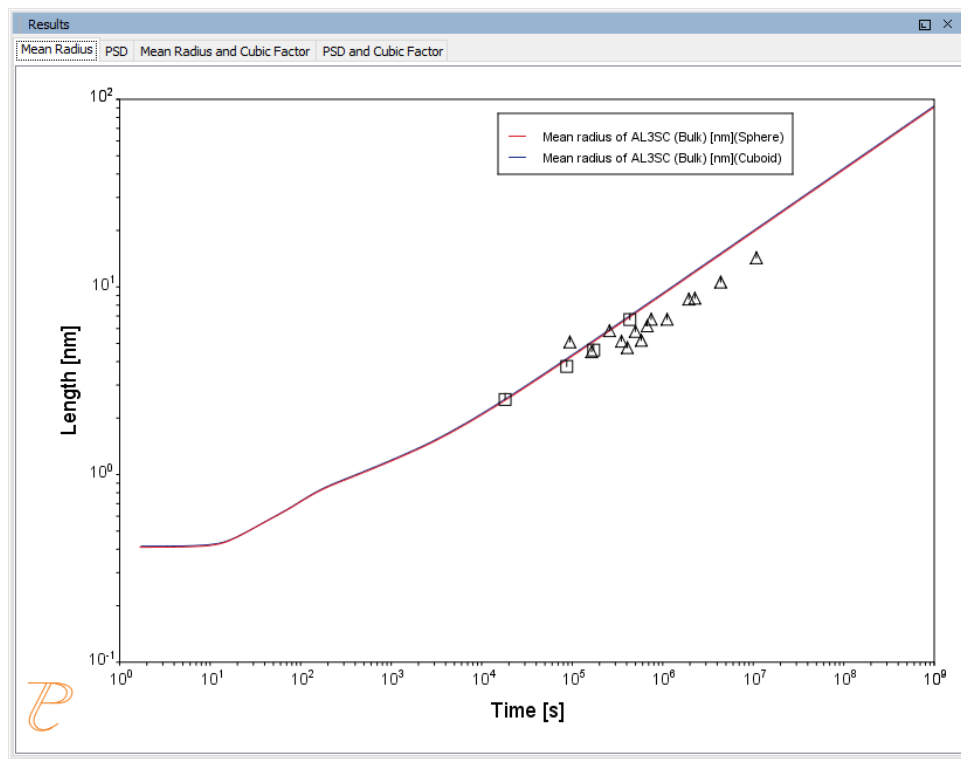
To ensure that the settings are done on the correct Precipitation Calculators, the **Sphere** and **Cuboid** nodes are renamed from **Precipitation Calculator** to match their morphology. The morphology is set in the **Precipitate Phase** section when you click **Show details**. See P_08 for an example of this.

| System (System Definer) | |
|---------------------------------------------------------|-----------------------------------------------|
| Database package | Demo: Aluminum-based alloys (ALDEMO, MALDEMO) |
| Elements | Al, Sc |
| Sphere and Cuboid Conditions (Precipitation Calculator) | |
| Composition | Al-0.18Sc Mole percent |
| Matrix phase | FCC_A1 |

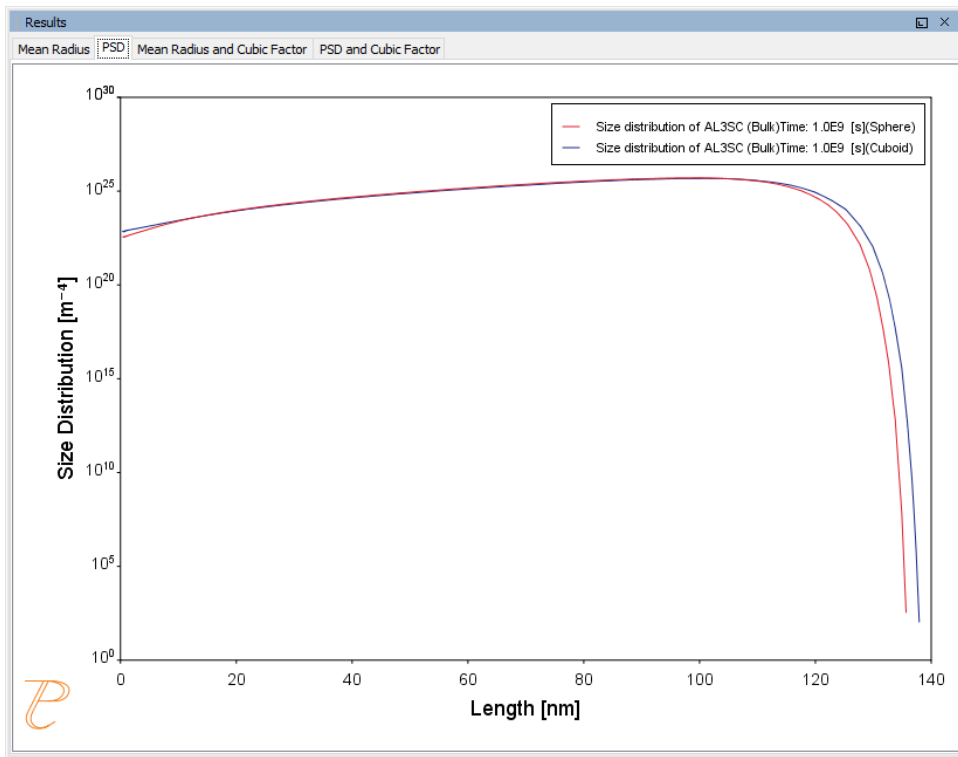
| | |
|---------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Precipitate phase | AL3SC |
| Matrix Phase Data Parameters (Precipitation Calculator) | |
| Elastic properties (click Show details to display this setting) | <p>For the Sphere node (renamed from Precipitation Calculator), the default, Disregard is kept.</p> <p>For the Cuboid node (renamed from Precipitation Calculator), choose Cubic. Then enter the elastic constants accordingly. Default elastic constants are given based on the major element of the alloy system. In this example that is</p> <ul style="list-style-type: none"> • c11 is 108.2 GPa • c12 is 61.3 GPa • c44 is 28.5 GPa |
| Precipitate Phase Data Parameters (Precipitation Calculator) | |
| Nucleation sites | Bulk |
| Interfacial energy | The default |
| Morphology (click Show details to display this setting) | <p>For the Sphere node (renamed from Precipitation Calculator), keep the default.</p> <p>For the Cuboid node (renamed from Precipitation Calculator), Cuboid is selected.</p> |
| Transformation strain (click Show details to display this setting) | <p>For the Sphere node (renamed from Precipitation Calculator), keep the default.</p> <p>For the Cuboid node (renamed from Precipitation Calculator), Calculate from molar volume is selected to obtain a purely dilatational strain.</p> |
| Calculation Type (Precipitation Calculator) | |
| Calculation type | Isothermal |
| Temperature | 350° C |
| Simulation time | 1.0E9 seconds |
| Datasets (Experimental File Reader) | |
| Dataset 1 and Dataset 2 | Data sets included with this example and imported to one Experimental File Reader. It is used for the Mean Radius plot. |

PLOT RESULTS

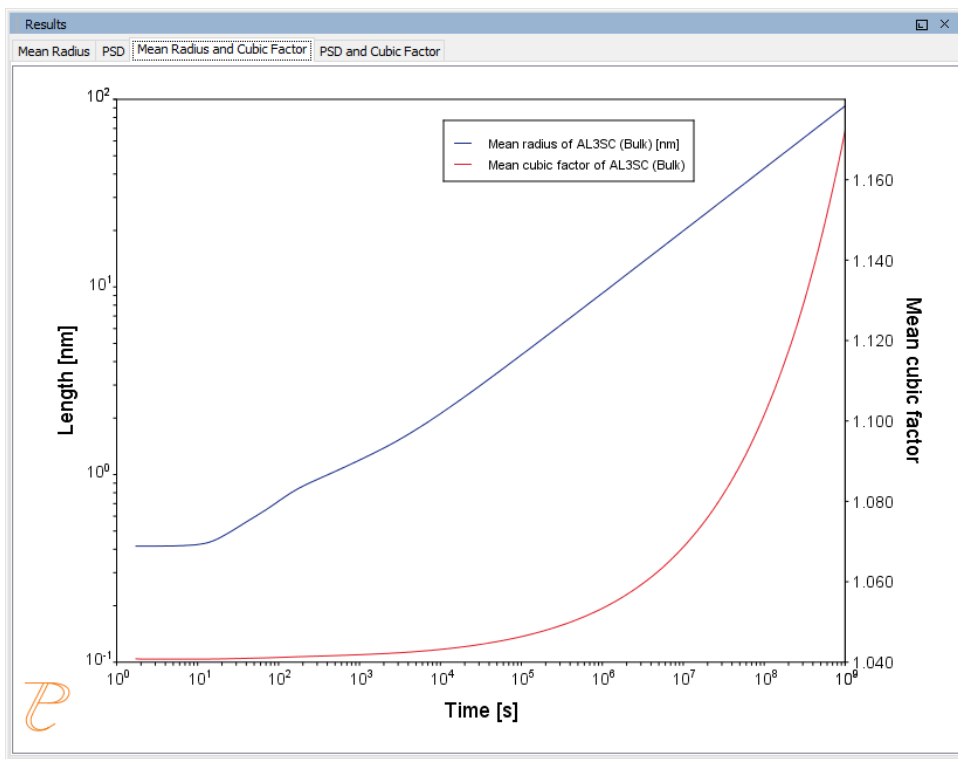
Mean Radius



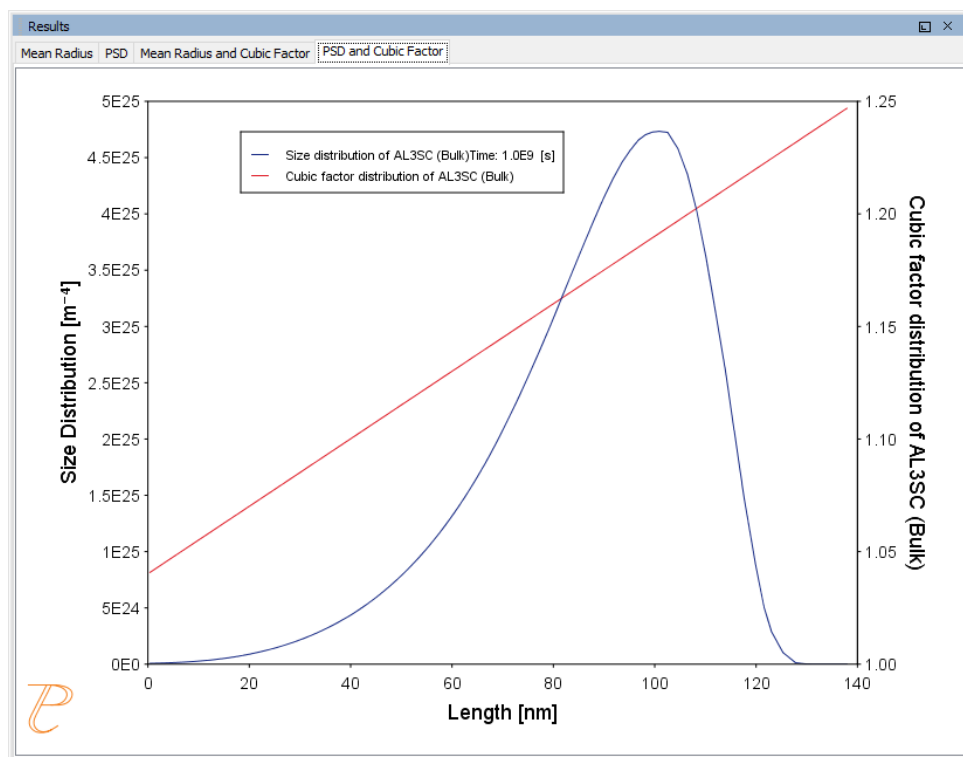
PSD



Mean Radius and Cubic Factor



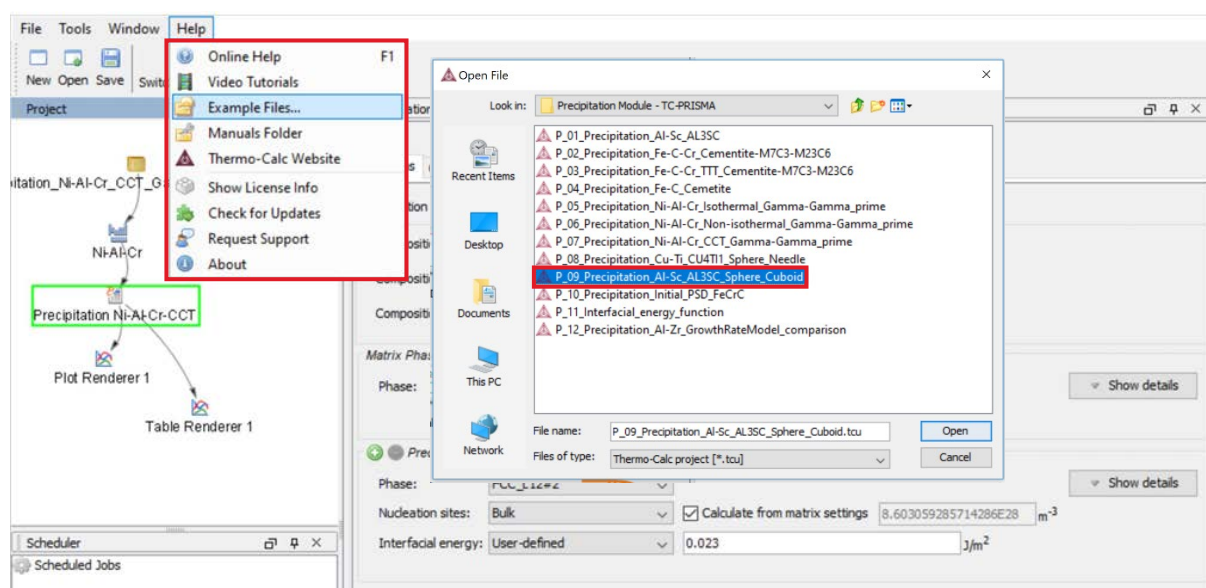
PSD and Cubic Factor



Precipitation of Al-Sc AL3SC with Assumption of Sphere and Cuboid Morphologies: Precipitation Example P_09

HELPFUL INFORMATION

- **All users can run this calculation**, even those who do not have a license for the Precipitation module (TC-PRISMA).
- **A companion video** is available for this example, which can be watched here:
https://www.youtube.com/playlist?list=PLfv6McToaTGSpgvuLoY3b_UV-8xpgLUKj
- This calculation is based on Precipitation module example *P_09 – Precipitation_Al-Sc_AL3SC_Sphere_Cuboid*, which is included in your installation. To run the example file, open Thermo-Calc and select **Help > Examples Files**. Open the *Precipitation module (TC-PRISMA)* folder. Double-click the example file and click **Perform** at the bottom centre of the **Configuration** window in Thermo-Calc.



ABOUT THE EXAMPLE

This example shows you how to calculate the precipitation of Al₃Sc phase from FCC_A1 matrix phase in an Al-Sc binary alloy using the Precipitation module (TC-PRISMA).

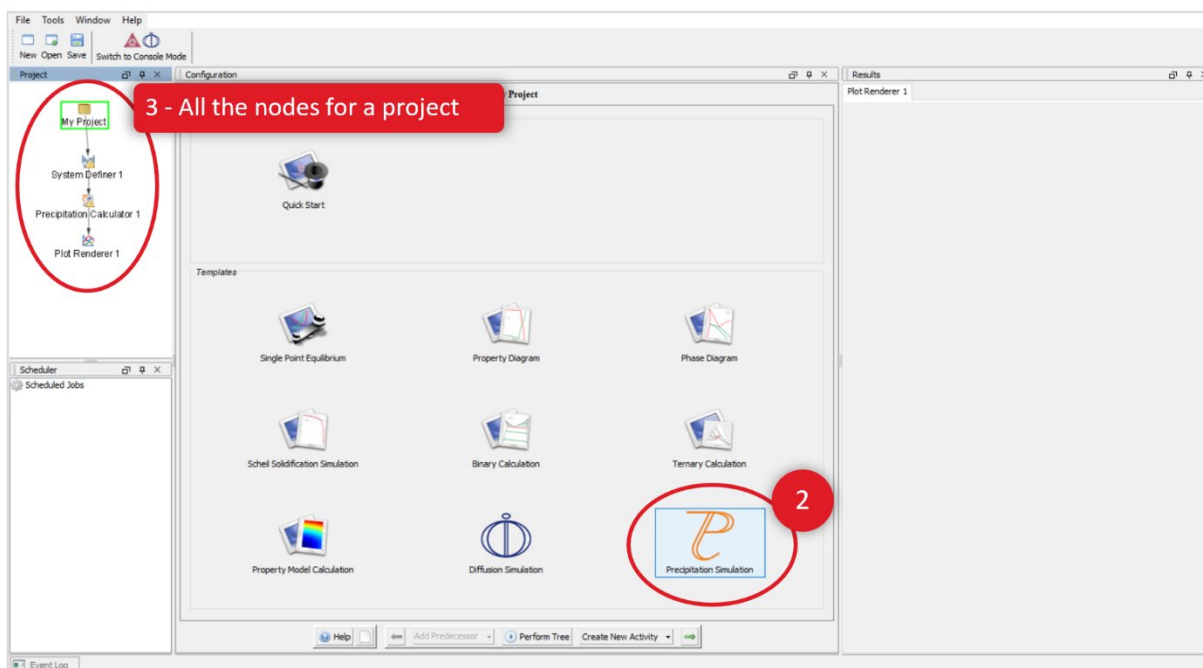
Two separate calculations are performed so you can make a comparison of the results, one assuming spherical morphology without elastic strain energy, and the other assuming cuboid morphology whose shape is determined by competition between interfacial energy and elastic strain energy.

In addition, mean cubic factor and cubic factor distribution are plotted for cuboid shape to illustrate the spherical-cuboidal transition during precipitation.

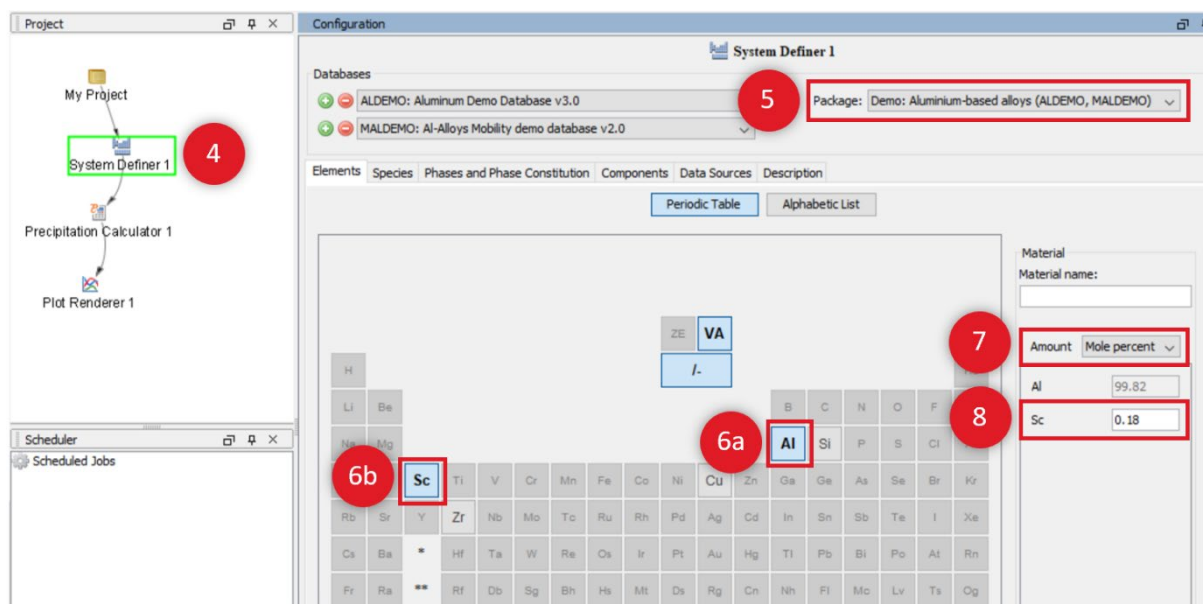
If you run the example file included in your software, the simulation results are compared with experimental data collected from Marquis and Seidman (2001) and Novotny and Ardell (2001).

SETTING UP THE SYSTEM

1. Open Thermo-Calc in Graphical Mode.
2. Under templates, click **Precipitation Simulation**.
3. All the nodes for a precipitation calculation are added to the **Project** window:



4. Click the **System Definer 1** node.
5. Set the database package to **DEMO: Aluminium based alloys**, which loads both thermodynamic and kinetic demonstration aluminium databases.
6. From the periodic table, select the elements **Al** (aluminium) then **Sc** (scandium). Be sure to select Al first so that it is the dependant element.
7. Just to the right of the periodic table, select **Mole Percent** as the **Amount**.
8. Enter 0.18 for **Sc**. This automatically sets **Al** to 99.82.



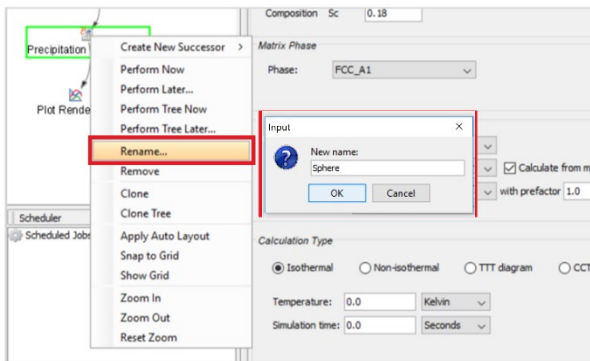
Our system is now defined, so we will set up the precipitation calculations.

SETTING UP THE PRECIPITATION CALCULATIONS

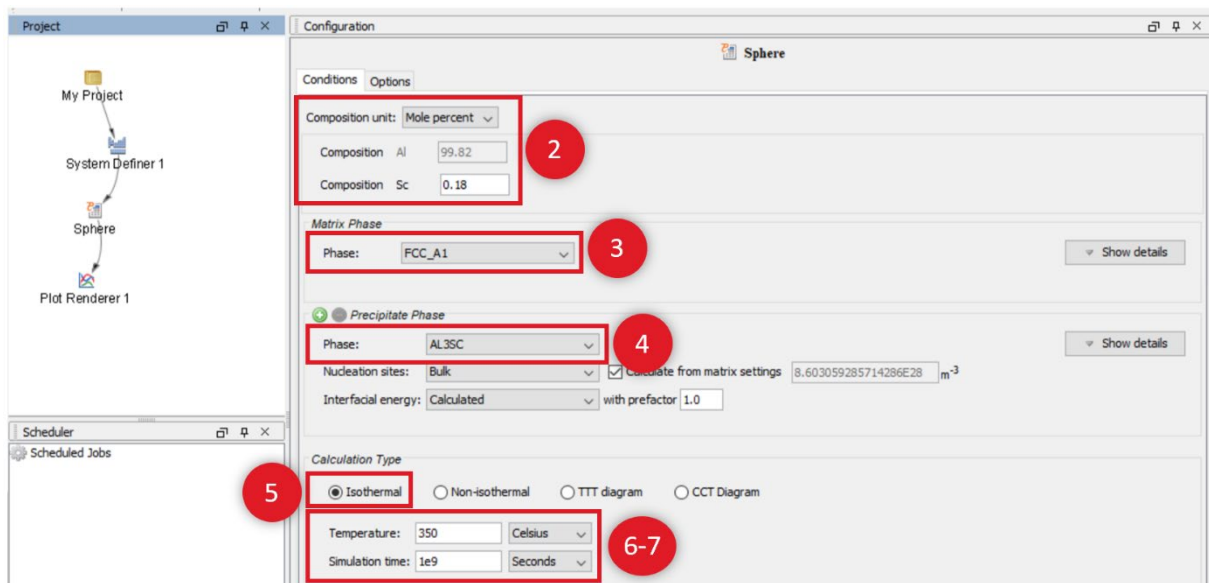
We will have two precipitation calculations in this example, one assuming spherical morphology without elastic strain energy, and the other assuming cuboid morphology whose shape is determined by competition between interfacial energy and elastic strain energy. We will then compare the results of the two calculations.

Setting up the Precipitation Calculation with Spherical Morphology

1. In the **Project** window, right-click the **Precipitation Calculator 1** node and select **Rename**. Enter **Sphere**, then press enter or click **OK**.



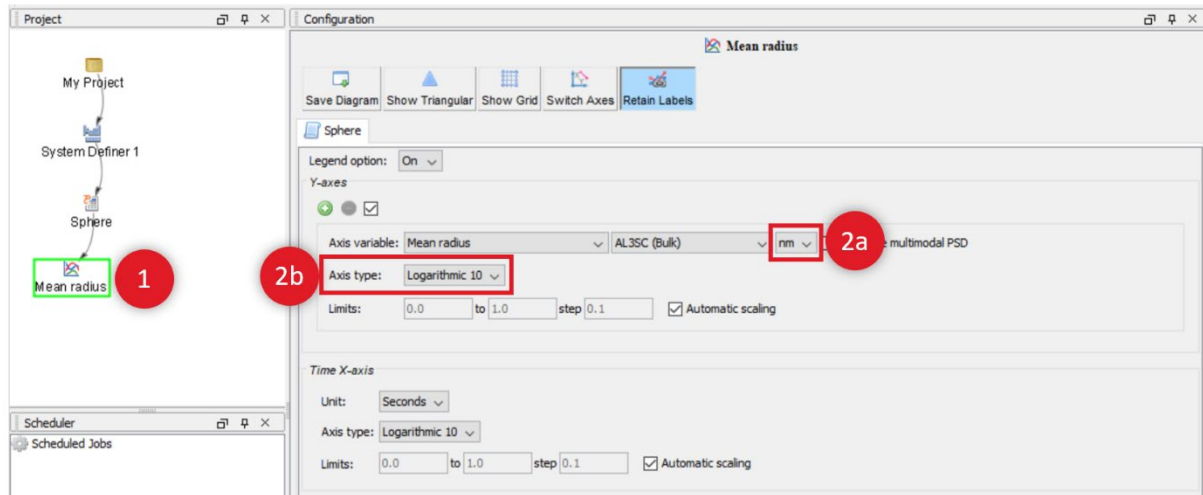
2. Notice that the composition we set in the **System Definer** auto-populated here.
3. Under **Matrix Phase** from the **Phase** list select **FCC_A1**.
4. Under **Precipitate Phase** from the **Phase** list select **AL3SC**.
5. Under **Calculation Type**, select **Isothermal**, which means that the same temperature is maintained throughout the calculation.
6. Enter 350 as the **Temperature** and select **Celsius**.
7. Enter 1.0E9 as the **Simulation time** and select **Seconds**.



Our first calculation is set, so we will configure the plot.

Configuring the Plot

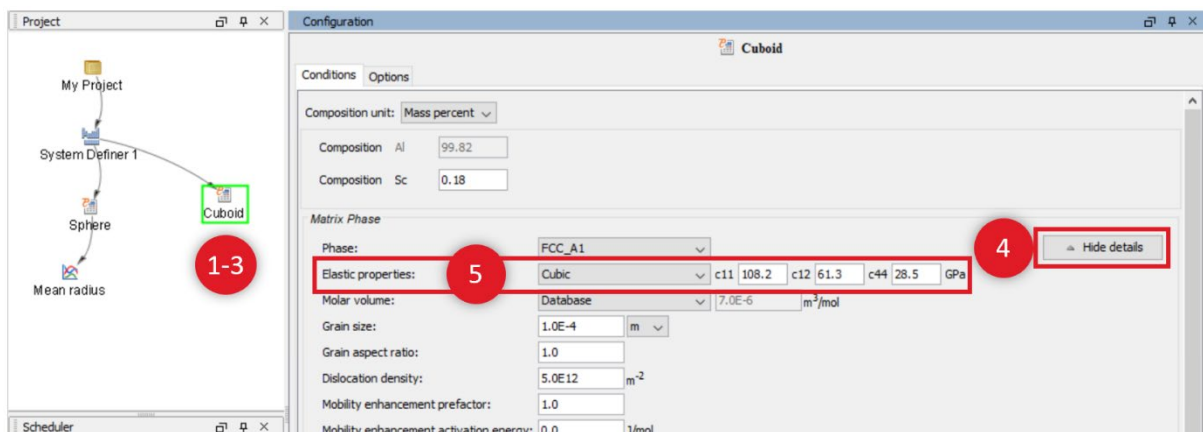
1. In the **Project** window, right-click **Plot Renderer 1** and select **Rename**. Name the plot Mean radius then press enter or click **OK**.
2. Under **Y-axes**, change the units to **nm** (nanometres) and from the **Axis type** list select **Logarithmic 10**.



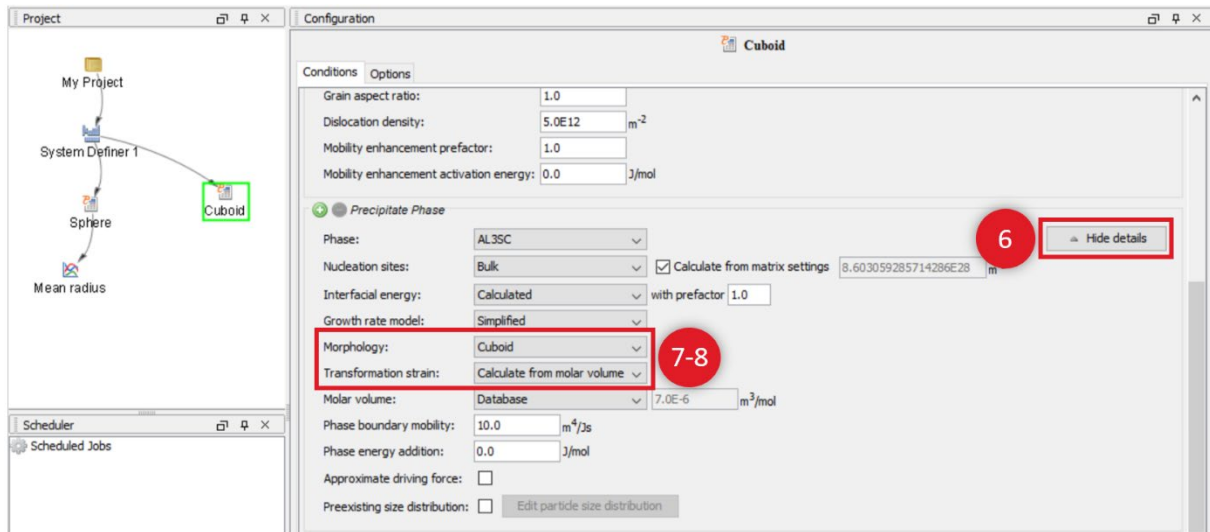
The plot is now set, but we will set up another calculation and link it to the same plot renderer before we run the simulation.

Setting up the Precipitation Calculation with Cuboid Morphology

1. In the **Project** window, right-click the **Sphere** node and select **Clone**.
2. Right-click the new calculator node and select **Rename**.
3. Name the node **Cuboid** and click **OK**.
4. On the **Configuration** window to the right of **Matrix Phase** click **Show Details**.
5. From the **Elastic Properties** list select **Cubic**. The program automatically suggests a good set of default values, so we will leave them as they are.



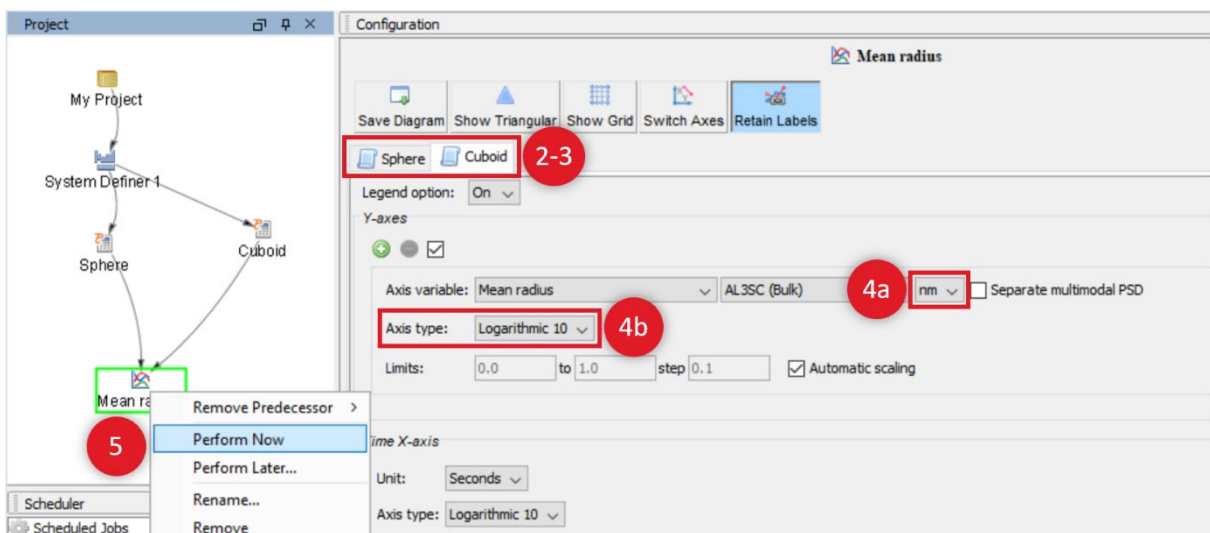
6. To the right of **Precipitate Phase**, click **Show Details**.
7. From the **Morphology** list select **Cuboid**.
8. From the **Transformation strain** list select **Calculate from molar volume**.



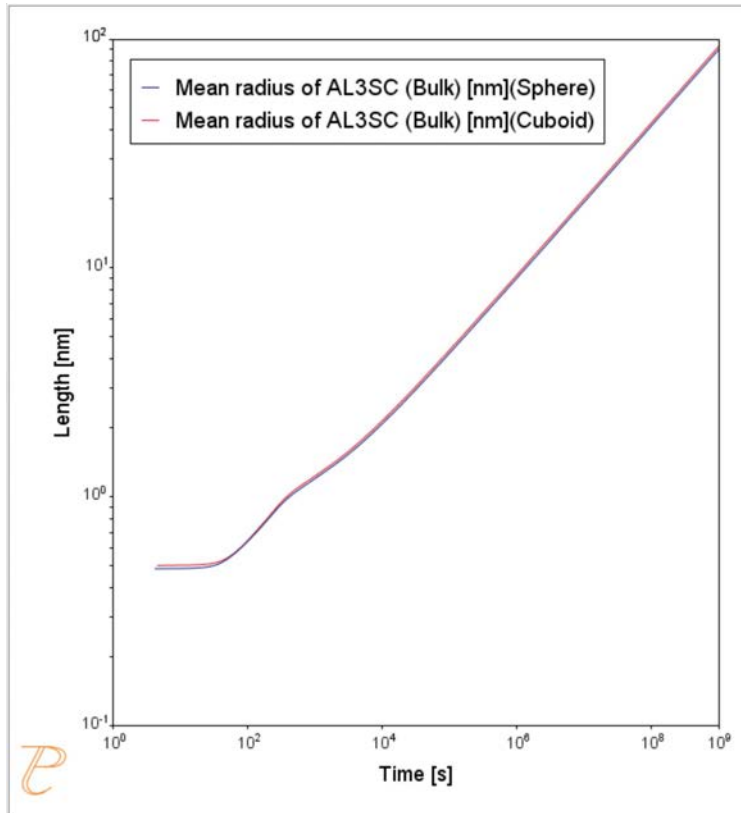
The second calculation is now set up, so we will link it to the Plot Renderer node.

Linking the Plot to the Calculation with Cuboid Morphology

1. In the **Project** window, right-click the **Mean radius** node and select **Add Predecessor >Cuboid**.
2. Notice that in the **Configuration** window there are two tabs associated with this plot, one for **Sphere** and one for **Cuboid**. We already configured the Sphere settings, so we just need to set up the Cuboid tab.
3. Click the **Cuboid** tab.
4. Under **Y-axes**, change the unit to **nm** (nanometers) and from the **Axis type** list select **Logarithmic 10**.
5. Our calculation is now ready, so right-click the **Mean radius** node and select **Perform Now**.



INTERPRETING THE RESULTS OF THE PRECIPITATION CALCULATIONS



In this plot, the blue line represents the sphere calculation and the red line represents the cuboid calculation. You can see that, in this instance, they are almost identical.

In this plot, the blue line represents the sphere calculation and the red line represents the cuboid calculation. You can see that, in this instance, they are almost identical.

By 'radius for non-spherical particles' we mean the radius of equivalent spheres with the same volume.

If you run the example file that is included in your software, the plot also contains an experimental file, which you can see closely matches the calculations.

PLOTTING ADDITIONAL VARIABLES

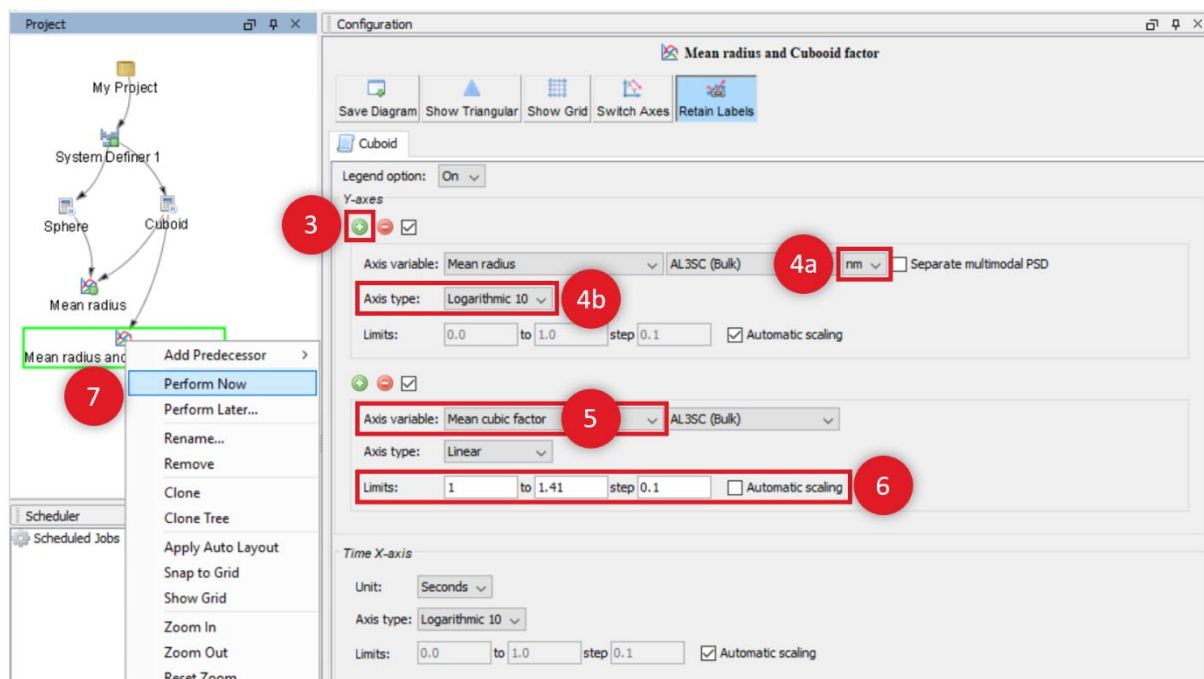
We will now use the same calculation to set up additional plots using the many plot variables that are available in the program. The examples below include two Y-axes each.

Plotting Mean Radius and Cuboid Factor

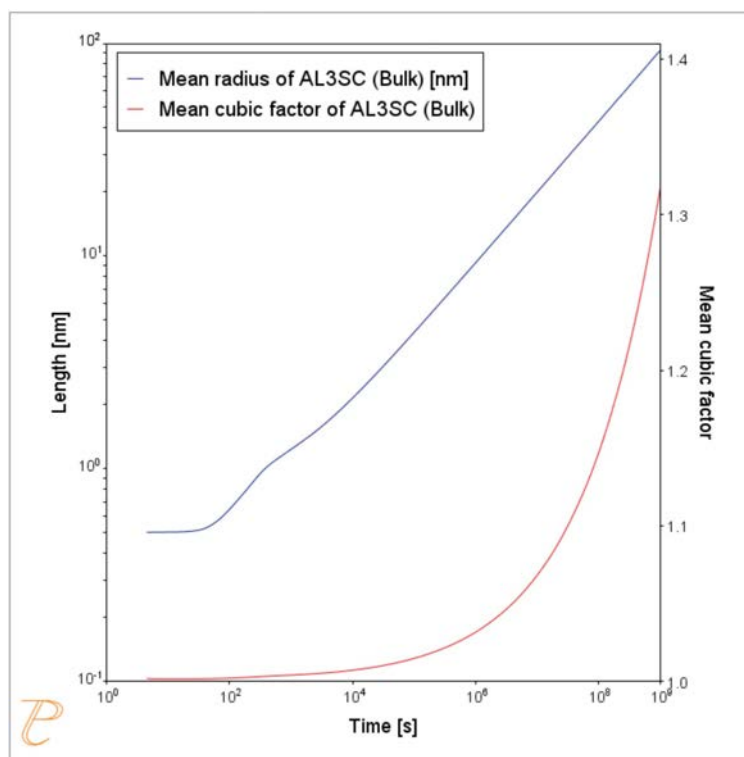
This plot will have two Y-axes: Mean radius and Cuboid factor.

1. Right-click the **Cuboid** node and add a **Plot Renderer**.
2. Right-click the new node and rename it **Mean radius and Cuboid factor**.
3. Under **Y-axes** click the green plus sign to add another axis.
4. Leave the first axis variable as *Mean radius*, but change the units to **nm** (nanometers) and set the axis type to **Logarithmic 10**.
5. Set the second **Axis variable** to **Mean cubic factor**.
6. Click to clear the **Automatic Scaling** check box. In the fields, enter the **Limits** from 1 to 1.41 and the **step** to 0.1.

7. The plot is now set, so right-click the **Mean radius and Cuboid factor** node and select **Perform Now**.



Interpreting the Results of Mean Radius and Cuboid Factor



In this plot, the blue line represents the evolution of the average radius of the cubic particles as a function of time. The red line shows the average cubic factor as a function of time.

The blue line represents the evolution of the average radius of the cubic particles as a function of time. Again, for non-spherical precipitates this means the radius of equivalent spheres with the same volume.

The red line shows the average cubic factor as a function of time. A value of one represents a spherical shape. A square root of two represents a cubic shape.

The evolution of the shape when the particles grows is determined by competition between interfacial energy and elastic strain energy. In general the shape is close to spherical at small particle sizes because the interfacial energy term dominates.

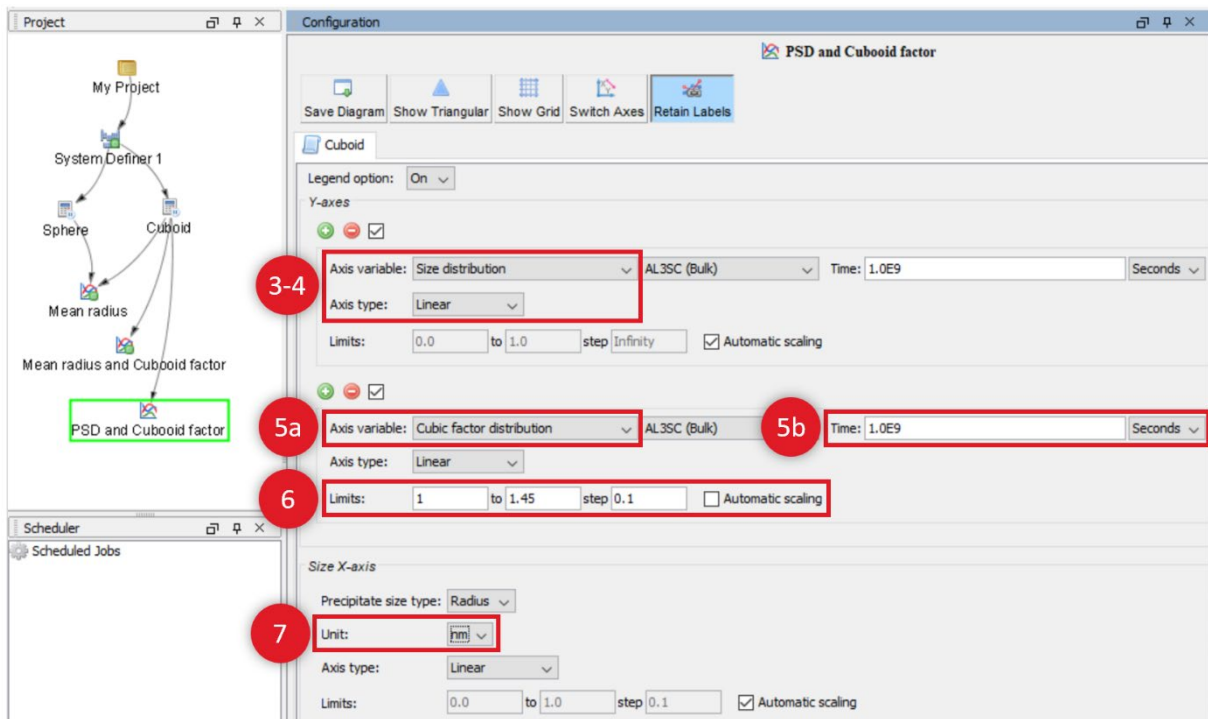
At large sizes the elastic energy dominates and it is therefore more favourable with a non-spherical shape. We can see that the particles get a more cubic form at later times when they grow to larger sizes.

Plotting Particle Size and Cubic Factor Distribution

This final plot will show the particle size and cubic factor distribution at the end of the simulation.

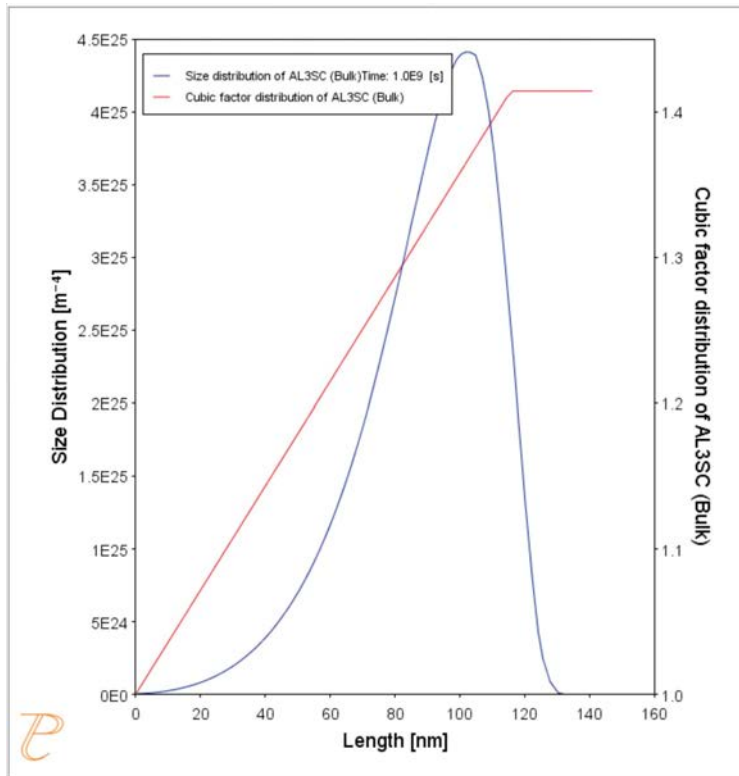
This plot will also have two Y-axes, so we will clone the previous plot.

1. Right-click the **Mean radius and Cuboid factor** node and select **Clone**.
2. Right-click the new node and rename it **PSD and Cuboid factor**.
3. Under the **Y-axes**, select **Size Distribution** as the first **Axis variable**.
4. Change the **Axis type** to **Linear**.
5. Set the second Y-axis to **Cubic factor distribution** and enter a **Time** of **1e9 Seconds**.
6. Click to clear the **Automatic Scaling** check box. Enter the **Limits** from 1 to 1.45 and the **step** to 0.1.
7. Under **Size X-axis**, change the unit to **nm** (nanometers).
8. Click **Perform** at the bottom centre of the **Configuration** window.



The screenshot shows the Thermo-Calc software interface. On the left, the 'Project' tree shows a hierarchy: 'My Project' -> 'SystemDefiner 1' -> 'Sphere' and 'Cuboid' -> 'Mean radius' and 'Mean radius and Cuboid factor'. A new node 'PSD and Cuboid factor' is highlighted in green. On the right, the 'Configuration' window is open for 'PSD and Cuboid factor'. It has tabs for 'Save Diagram', 'Show Triangular', 'Show Grid', 'Switch Axes', and 'Retain Labels'. The 'Cuboid' tab is active. Under 'Legend option', 'On' is selected. Under 'Y-axes', there are two axes. The first axis is 'Size distribution' (AL3SC (Bulk)) with 'Time: 1.0E9' and 'Seconds'. The second axis is 'Cubic factor distribution' (AL3SC (Bulk)) with 'Time: 1.0E9' and 'Seconds'. Both axes have 'Axis type: Linear'. The first axis has 'Limits: 0.0 to 1.0 step Infinity' and 'Automatic scaling' checked. The second axis has 'Limits: 1 to 1.45 step 0.1' and 'Automatic scaling' unchecked. Under 'Size X-axis', 'Precipitate size type: Radius' is selected, 'Unit: nm' is selected, 'Axis type: Linear' is selected, and 'Limits: 0.0 to 1.0 step 0.1' with 'Automatic scaling' checked. Red circles and boxes highlight these settings: 3-4 for the first Y-axis configuration, 5a for the second Y-axis variable, 5b for the second Y-axis time, 6 for the second Y-axis limits and scaling, and 7 for the X-axis unit.

Interpreting the Results of Particle Size Distribution and Cuboid Factor



In this plot, the blue curve shows the particle size distribution and the red line shows the cubic factor distribution.

The blue curve, which shows the particle size distribution, is close to the regular LSW size distribution that we would have expected for spherical particles.

The cubic factor distribution shows that the smallest particles are closer to spherical and that the larger ones get more and more cubic.

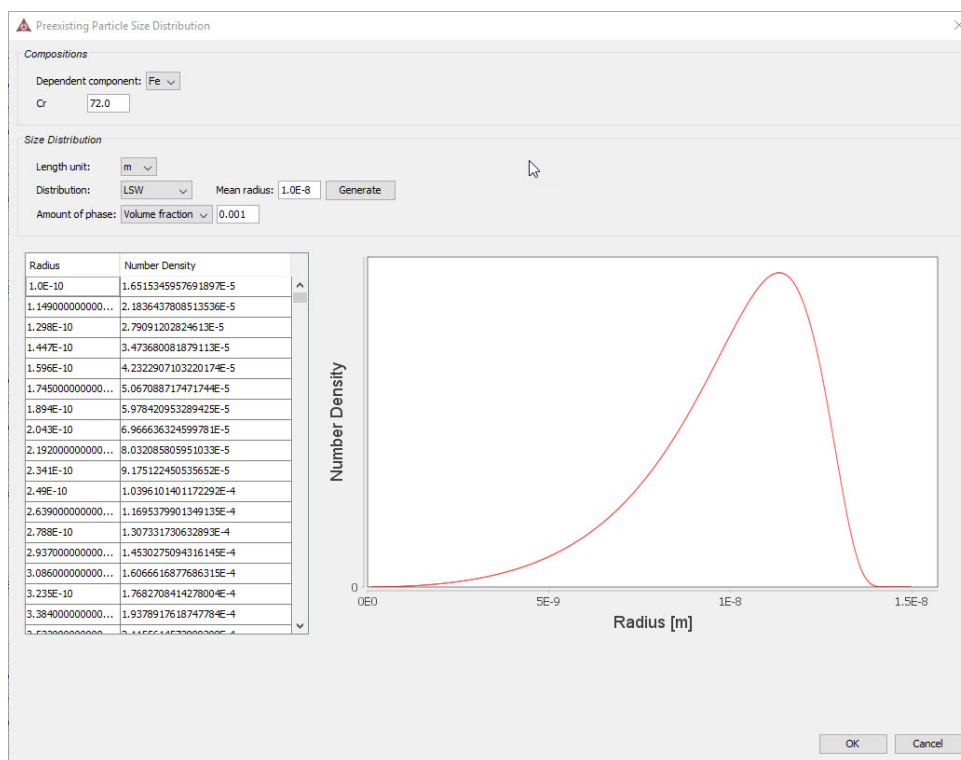
References

1. Marquis, E.A, and D.N Seidman. 2001. "Nanoscale Structural Evolution of Al3Sc Precipitates in Al(Sc) Alloys." *Acta Materialia* 49 (11): 1909–19.
2. Novotny, Gabriel M., and Alan J. Ardell. 2001. "Precipitation of Al3Sc in Binary Al–Sc Alloys." *Materials Science & Engineering, A: Structural Materials: Properties, Microstructure and Processing* 318 (1–2): 144–54.

P_10: Initial Particle Size Distribution of Fe-Cr-C

This example demonstrates the effect of initial particle size distribution of the precipitate phases on the overall precipitation kinetics. It uses two Precipitation Calculators to simulate and compare carbide precipitations from a ferritic BCC_A2 matrix in a Fe-0.1C-12Cr alloy. Three carbides, CEMENTITE, M23C6 and M7C3, are included in the calculations for competitive precipitations, and the precipitation kinetics are compared with or without initial particle size distribution.

The example illustrates the use of the particle size distribution setting. You can import data from a spreadsheet or text file (.xls, .xlsx, .csv or .txt formats are acceptable). The Preexisting Particle Size Distribution window shown below, provides a graphical representation of the radius versus corresponding frequencies.



PROJECT FILE AND VIDEO TUTORIAL INFORMATION

- Folder: Precipitation Module - TC-PRISMA
- File name: P_10_Precipitation_Initial_PSD_FeCrC.tcu



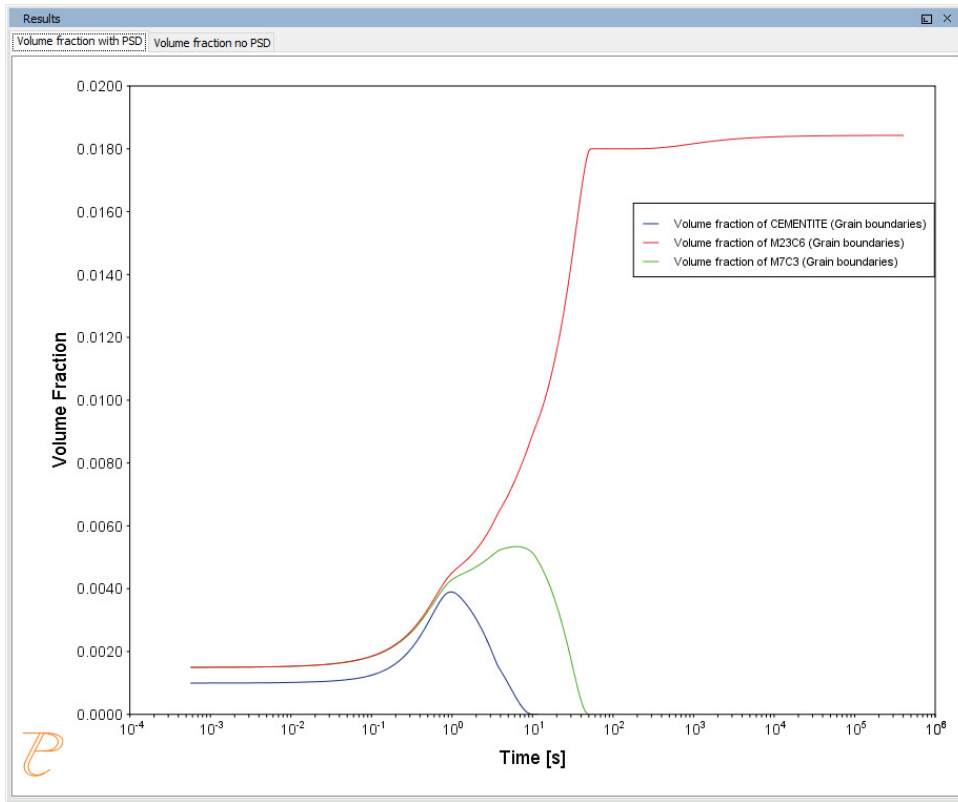
Also see [our website](#) and [YouTube channel](#) for other examples of the Precipitation Module.

EXAMPLE SETTINGS

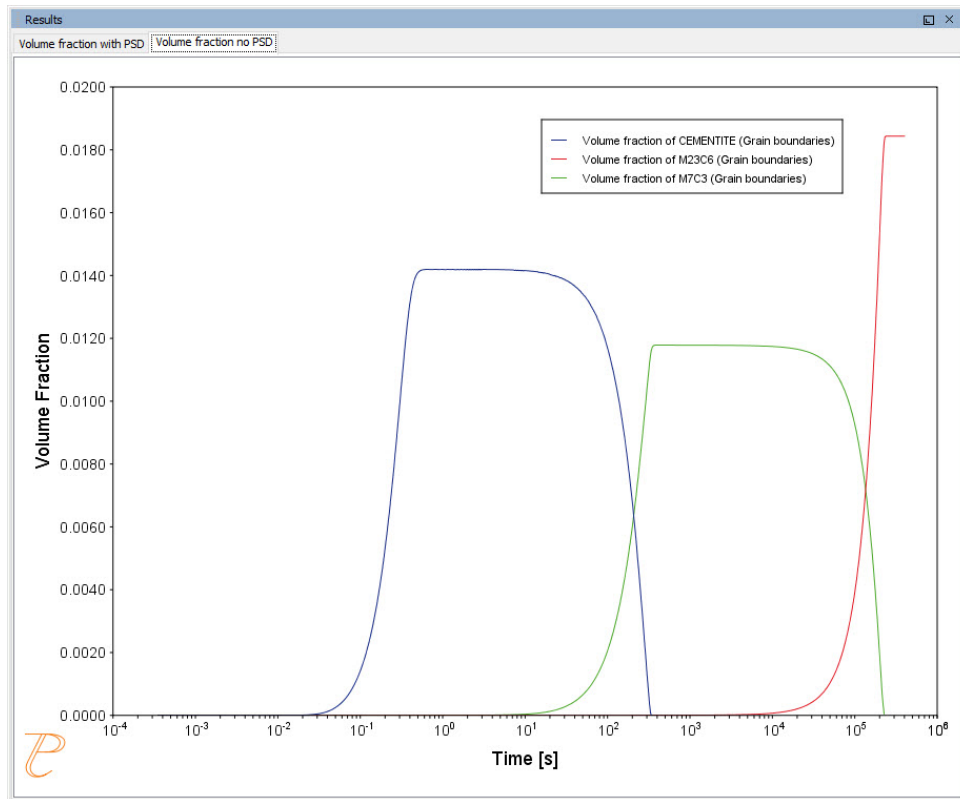
| System (System Definer) | |
|-----------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Database package | Demo: Steels and Fe-alloys (FEDEMO and MFEDEMO) |
| Elements | Fe, C, Cr |
| Conditions (Precipitation Calculator) | |
| Composition | Fe-0.1C-12Cr Mass percent |
| Matrix phase | BCC_A2 All other defaults are kept. |
| Precipitate phases | CEMENTITE, M23C6 and M7C3 |
| Precipitate Phase Data Parameters (Precipitation Calculator) | |
| Nucleation sites | Grain boundaries (all calculations): Calculated from the matrix settings with a wetting angle of 90° |
| Interfacial energy | User-defined function $f(r,T)$ (all calculations): <ul style="list-style-type: none">• CEMENTITE: 0.167 J/m²• M23C6 0.252 J/m²• M7C3 0.282 J/m² |
| Preexisting size distribution (click Show details to display this setting) | <p>For the Precipitation Calculator including particle size distribution, and for all precipitate phases, this check box is selected.</p> <p>For each precipitate phase (CEMENTITE, M23C6 and M7C3), click Edit particle size distribution to make changes to the parameters. A window opens with a graphical representation of the radius vs number density.</p> |
| Calculation Type (Precipitation Calculator) | |
| Calculation type | Isothermal |
| Temperature | 1053 K |
| Simulation time | 400 000 seconds |

PLOT RESULTS

Volume Fraction with Initial Particle Size Distribution



Volume Fraction with No Initial Particle Size Distribution



P_11: Interfacial Energy Function

In some cases, interfacial energy may be a function of temperature and/or particle radius. This example uses four Precipitation Calculators at four temperature points in 30 K increments: 673 K, 703 K, 733 K, and 763 K. It is an isothermal calculation to examine the mean radius of an Al-0.12Sc system. It uses an FCC_A1 matrix phase and Al3Sc precipitate phase with bulk nucleation sites and user-defined interfacial energy function. The user defined interfacial energy function uses an error function to set a smooth transition of the interfacial energy from 0.065 J/m² to 0.085 J/m² for particle radii below and above 1e-8m and 5e-8m, respectively.

A dataset based on Iwamura and Miura (¹) data is compared with the calculated results.

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

- Folder: Precipitation Module - TC-PRISMA

1. Iwamura, S, and Y Miura. 2004. "Loss in Coherency and Coarsening Behavior of Al3Sc Precipitates." *Acta Materialia* 52 (3): 591–600.

- File name: *P_11_Interfacial_energy_function.tcu*



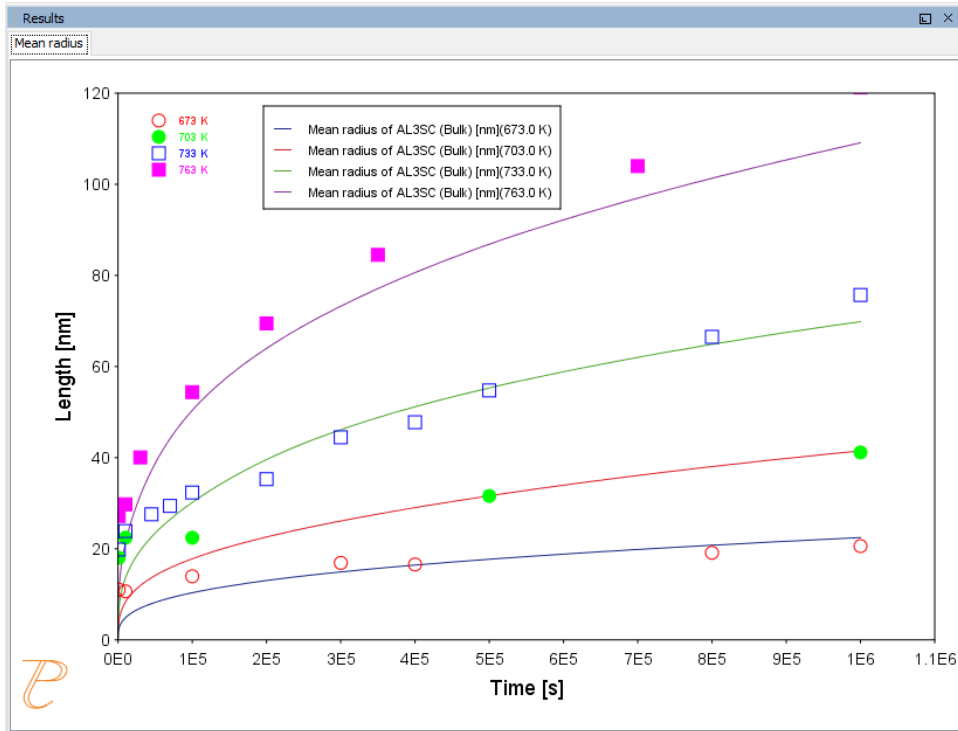
Also see [our website](#) and [YouTube channel](#) for other examples of the Precipitation Module.

EXAMPLE SETTINGS

| System (System Definer) | |
|---------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Database package | Demo: Aluminum-based Alloys (ALDEMO, MALDEMO) |
| Elements | Al, Sc |
| Conditions (Precipitation Calculator) | |
| Composition | Al-0.12Sc Mole percent |
| Matrix phase | FCC_A1 All other defaults are kept. |
| Precipitate phase | AL3SC Nucleation sites (all calculations): Bulk ($6.025 \times 10^{28} \text{ m}^{-3}$) Interfacial energy (all calculations): User-defined function $f(r,T)$: $0.075 + 0.011 \cdot \text{erf}((r - 3 \times 10^{-8}) / 1 \times 10^{-8} \text{ J/m}^2)$ |
| Calculation Type (Precipitation Calculator) | |
| Calculation type | Isothermal (all calculations) |
| Temperature | Four temperature points in 30 K increments: 673 K, 703 K, 733 K, and 763 K. |
| Simulation time | 1 000 000 seconds (all calculations) |
| Datasets (Experimental File Reader) | |
| Wamura 2004 (Dataset 1) | Data set included with this example and imported to one Experimental File Reader. |

PLOT RESULTS

Mean Radius



P_12: Comparing Growth Rate Models for an Al-Zr System

This example compares the **Simplified**, **General** and **Advanced** growth rate models for an Al-Zr system. The resulting plot compares the mean radius of the spheres for each AL3ZR_D023 precipitate phase calculated for each type of growth rate model.



The example takes several minutes to run.

All models treat a spherical particle (precipitate) of stoichiometric composition or with negligible atomic diffusivity. Local equilibrium at the precipitate-matrix interface is assumed.

When you use the *Advanced* model, the velocity of a moving phase interface and the operating tie-line are solved together from flux-balance equations. This model can treat both high supersaturation and cross diffusion rigorously. It can also capture the transition between NPLE (non-partitioning local equilibrium) and PLE (partitioning local equilibrium) without any *ad hoc* treatment.

The *Simplified* model is based on the quasi-steady state diffusion approximation, and estimates solute partitioning with matrix composition and nuclei composition instead of time-consuming stepwise tie-line calculations. It also neglects cross diffusion for simplicity.

The *General* model can be considered the same theoretical approximation as, but an improvement over, the *Simplified* model, with cross-diffusion terms taken into account, as well as adjustment of Gibbs-Thomson effect and effective diffusivity implemented.

A dataset based on Knippling et al. (¹) data is compared with the calculated results.

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_12_Precipitation_Al-Zr_GrowthRateModel_comparison.tcu*



Also see [our website](#) and [YouTube channel](#) for other examples of the Precipitation Module.

EXAMPLE SETTINGS

| System (System Definer) | |
|---------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|
| Database package | Demo: Aluminum-based Alloys (ALDEMO, MALDEMO) |
| Elements | Al, Zr |
| Conditions (Precipitation Calculator) | |
| Composition | Al-0.2Zr Mole percent |
| Matrix phase | FCC_A1 All other defaults are kept. |
| Precipitate phase | AL3ZR_D023 Click Show details to select the Growth rate model (Simplified, Advanced and General) . All other defaults are kept. |
| Calculation Type (Precipitation Calculator) | |
| Calculation type | Isothermal |
| Temperature | 425 Celsius |

1. Knippling, Keith E., David C. Dunand, and David N. Seidman. 2008. "Precipitation Evolution in Al–Zr and Al–Zr–Ti Alloys during Isothermal Aging at 375–425°C." *Acta Materialia* 56 (1): 114–27. doi:10.1016/j.actamat.2007.09.004.

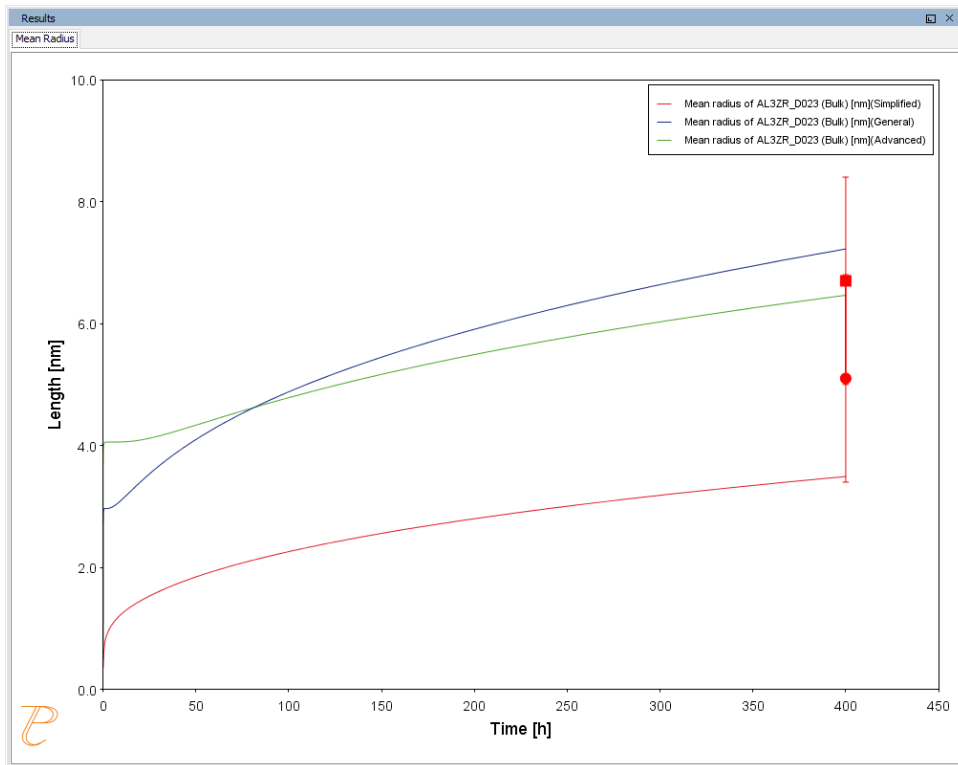
Simulation time | 400 hours

Datasets (Experimental File Reader)

2008 Knipling | Data set included with this example and imported to one Experimental File Reader.

PLOT RESULTS

Mean Radius



P_13: Paraequilibrium Precipitation of Cementite Fe-C-Cr

In this example, the precipitation of cementite during tempering of a Fe-Cr-C steel is simulated considering two interface conditions: one is the usual ortho-equilibrium condition; the other is the para-equilibrium condition. The simulation results are compared with the experimental data from Sakuma et al (1980) T. Sakuma, N. Watanabe, and T. Nishizawa, "The effect of alloys element on the coarsening behavior of cementite particles in ferrite", *Trans. JIM*, v. 21, 1980, pp.159-168..



The example may take over two hours to run.

This example demonstrates that the early stage of the cementite precipitation can only be accounted for by a simulation applying the para-equilibrium condition, under which the precipitation kinetics are controlled by the diffusion of C. The comparison also shows a later stage gradual transition from the para-equilibrium condition to the ortho-equilibrium condition, and if the tempering time is long enough the diffusion of Cr has a dominating effect on the coarsening of cementite.

PROJECT FILE AND VIDEO TUTORIAL INFORMATION

- Folder: Precipitation Module - TC-PRISMA
- File name: *P_13_Precipitation_Fe-C-Cr_Paraequilibrium_Precipitation_of_Cementite.tcu*



Also see [our website](#) and [YouTube channel](#) for other examples of the Precipitation Module.

EXAMPLE SETTINGS

| System (System Definer) | |
|---------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------|
| Database package | Demo: Steels and Fe-alloys (FEDEMO, MFEDEMO) |
| Elements | Fe, Cr, C |
| Conditions (Precipitation Calculator) | |
| Composition | Fe-0.95Cr-1.065C Mass percent |
| Matrix phase | BCC_A2 All other defaults are kept. |
| Precipitate phase | CEMENTITE Click Show details to select the Growth rate model (Simplified and Para-eq) . All other defaults are kept. |
| Calculation Type (Precipitation Calculator) | |
| Calculation type | Isothermal |
| Temperature | 773 Kelvin |

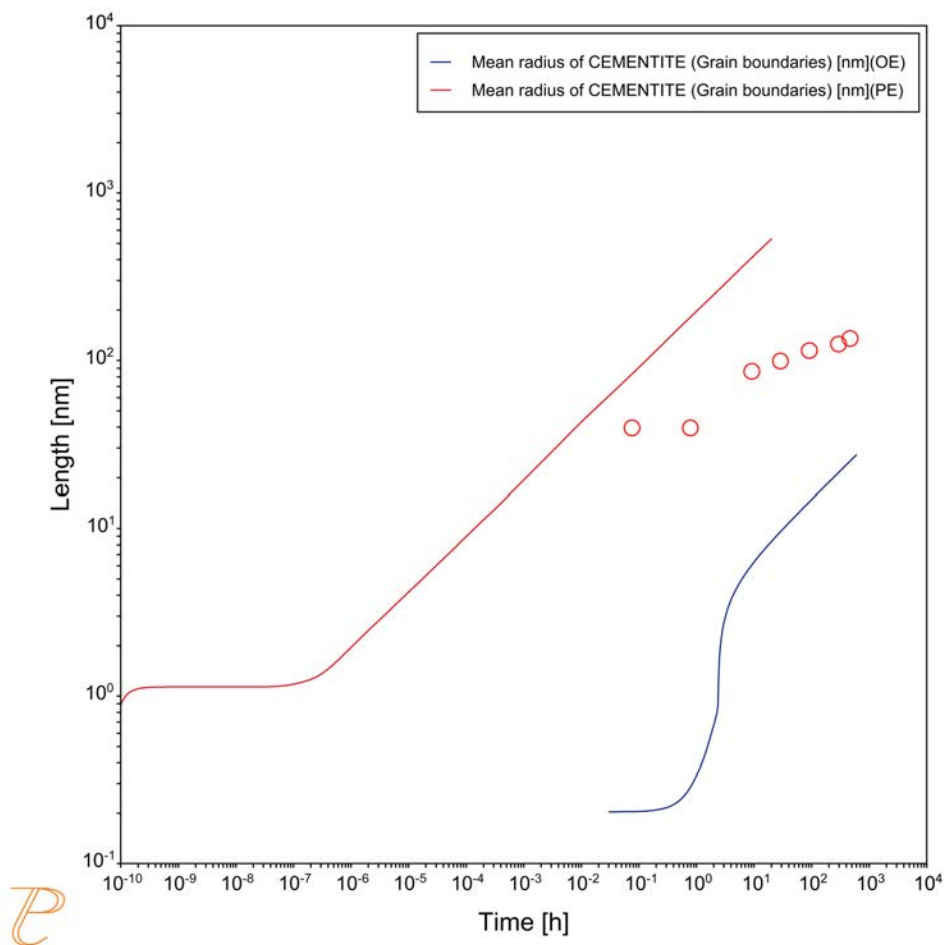
| | |
|-----------------|--------------------------------------------------------------------------------|
| Simulation time | 20 hours for the paraequilibrium model and 600 hours for the simplified model. |
|-----------------|--------------------------------------------------------------------------------|

Datasets (Experimental File Reader)

| | |
|-------------|-----------------------------------------------------------------------------------|
| 1980 Sakuma | Data set included with this example and imported to one Experimental File Reader. |
|-------------|-----------------------------------------------------------------------------------|

PLOT RESULTS

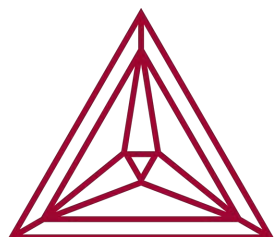
Mean Radius



Comparing results from Para-eq (PE) and Simplified (OE) growth models.

Thermo-Calc Property Model Development Framework

Thermo-Calc Version 2020a



Introduction to the Property Model Development Framework

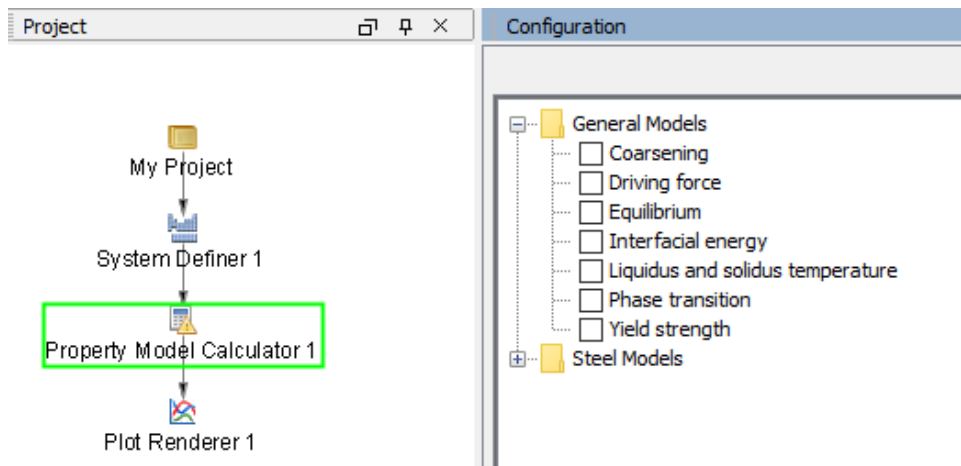


Only an overview is included here. Please use the standalone PDF or the Online Help for IDE and tutorial instructions. The PDF guide is available in the **Manuals** folder, accessible from the **Help** menu. There is also a subfolder containing the tutorial Python files.



This API is like a plug in to Thermo-Calc. It is not an SDK. That is, you cannot use this API to build other applications to work with Thermo-Calc like you would use the *TC-API* or the *TQ-Interface*.

The "[Property Model Calculator](#)" on page 75 in Thermo-Calc Graphical Mode has predefined models available for immediate use and new models are being added on a regular basis. The *Property Model Development Framework* enables you to create custom property models that are then able to be included with the Property Model Calculator and ultimately used for your simulations.



When you use the *Property Model Development Framework API*, it extends the software to enable you to create property models. The models are written in the easy-to-learn programming language **Python** and the API provides seamless integration into Thermo-Calc. This includes access to thermodynamic and kinetic calculation routines as well as to the Thermo-Calc plotting system.

The API is based on *Jython*, which is a Python implementation running in the Java Virtual Machine. All Python libraries that are compatible to the Jython distribution can be used within the model (but not libraries based on native C-code).



Model development is possible without any additional installation by using a text editor (for example *Notepad++*). However, it is recommended you use a Python Integrated Development Environment (IDE), which provides you with advanced features such as debugging and auto-completion.

Property Model Installation Directory



All property models (whether these are predefined or custom models) must be located in a subdirectory of the property model directory. You can go to **Tools** → **Options** and the **Model directory** field displays the default directory.

Predefined models included with the Property Model Calculator are installed in the locations below based on your operating system. If you create your own models, this is the default directory where these are saved. You can also use one of these as a template to create your own property model.

| Operating system | Property model installation directory |
|------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Windows | <code>C:\Users\<user>\Documents\Thermo-Calc\2020a\PropertyModels</code> |
| Linux | On Linux all user files are installed where the program is installed. If installed as root the default is: <code>/opt/Thermo-Calc/2020a/PropertyModels</code> |
| Mac | <code>/Users/Shared/Thermo-Calc/2020a/PropertyModels</code> |

Creating a Custom Property Model



There is a guide, including tutorials and the classes and methods of the API, available as a separate PDF, included with your installation (**Help>Manuals Folder**) and on our [website](#). It includes details of the API classes and methods and details about how to debug with an IDE.

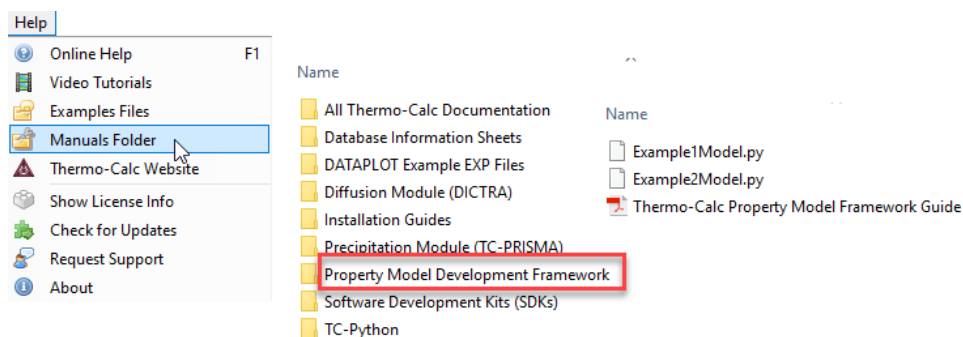
Example models demonstrating the most important features can be found in the tutorial examples included in the PDF Guide. The PDF includes the instructions and code you can copy. Example models are also in the property model directory.

A new property model can be created and modified at any time during a Thermo-Calc session. The model is automatically reloaded and you do not need to restart Thermo-Calc.

PROPERTY MODEL TUTORIALS

The tutorial Python files are available with your installation. These examples are also included with the PDF guide but placed in the installation folder to make it easier to copy the text and re-use it in your own Python files.

There is a PDF guide and tutorial examples included with your installation. In Thermo-Calc from the menu, select **Help → Manuals Folder**. Then double-click to open the **Property Model Development Framework** folder. This guide is also available on our [website](#).



Thermo-Calc Property Model Framework Documentation

Release 2020a

Thermo-Calc Software AB

Nov 25, 2019

CONTENTS

| | | |
|----------|---------------------------------------------------------------------------|-----------|
| 1 | Introduction | 1 |
| 1.1 | Thermo-Calc Custom Property Models | 1 |
| 1.2 | Architecture of the Python Property Model API | 1 |
| 1.3 | Call Events for the Property Model Methods | 2 |
| 2 | Installing Jython and Setting Up an IDE | 3 |
| 2.1 | Installing Jython | 3 |
| 2.2 | Setting up the IDE | 3 |
| 2.2.1 | IntelliJ IDEA | 3 |
| 2.2.2 | PyCharm | 4 |
| 3 | Creating a New Property Model | 5 |
| 4 | Tutorial | 7 |
| 4.1 | Example 1: A Basic Property Model with Thermodynamic Properties | 7 |
| 4.1.1 | Access to the Thermo-Calc System | 8 |
| 4.1.2 | Basic Information About the Model | 9 |
| 4.1.3 | Defining Input and Output Parameters | 9 |
| 4.1.4 | Performing the Calculations | 10 |
| 4.2 | Example 2: Property Model Using Apache Math | 12 |
| 5 | Debugging | 15 |
| 5.1 | Setting up IntelliJ IDEA / PyCharm for Debugging Models | 15 |
| 5.2 | Editing Your Model during a Thermo-Calc Session | 16 |
| 6 | Providing translations | 17 |
| 6.1 | Example | 17 |
| 6.2 | Java Properties-files | 17 |
| 7 | API Reference | 19 |
| 7.1 | PythonPropertyModel Interface | 19 |
| 7.2 | ResultQuantity | 20 |
| 7.3 | ThermoCalcCalculator | 21 |
| 7.4 | ThermoCalcSystem | 25 |
| 7.5 | UIBooleanComponent | 31 |
| 7.6 | UIComponent | 32 |
| 7.7 | UICompositionComponent | 33 |
| 7.8 | UIConditionListComponent | 33 |
| 7.9 | UIFloatComponent | 33 |
| 7.10 | UIGeneralListComponent | 34 |
| 7.11 | UIPhaseListComponent | 35 |

| | | |
|------|----------------------------------|----|
| 7.12 | UITemperatureComponent | 35 |
| 7.13 | JavaPropertyManager | 36 |

INTRODUCTION

1.1 Thermo-Calc Custom Property Models

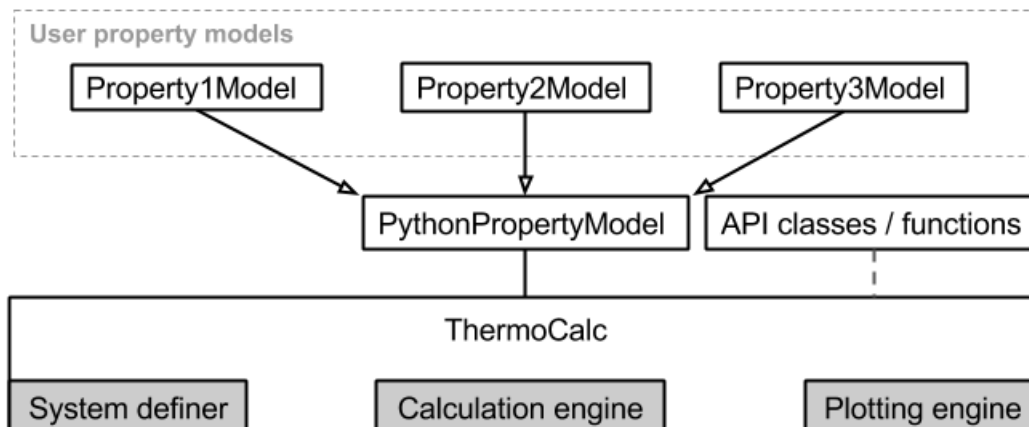
The *Python Property Model API* extends the Thermo-Calc software to enable you to create your own property models written in the easy-to-learn programming language **Python** and the API provides seamless integration of the property models into Thermo-Calc. This includes access to thermodynamic and kinetic calculation routines as well as to the Thermo-Calc plotting system.

The API is based on *Jython*, which is a Python implementation running in the Java Virtual Machine. All Python libraries that are compatible to the Jython distribution can be used within the model (but not libraries based on native C-code).

Model development is possible without any additional installation by using a text editor (for example *Notepad++*). However, using a Python Integrated Development Environment (IDE) provides you with advanced features such as debugging and auto-completion.

1.2 Architecture of the Python Property Model API

Every property model needs to contain a class that implements the interface *PythonPropertyModel*. It is the interface to the Thermo-Calc system and calculation engine and provides the calculation results to the Thermo-Calc plotting engine.



The basic building blocks of the property model API are:

- **ResultQuantity**: Defines a calculation result of a property model that will be provided by the property model after a model evaluation

classes: *ResultQuantity*

- **ThermoCalcCalculator:** Thermodynamic calculation engine of Thermo-Calc for the property models

classes: *ThermoCalcCalculator*

- **ThermoCalcSystem:** Provides all helper functionality within the property models to access the Thermo-Calc / GUI functionality

classes: *ThermoCalcSystem*

- **UIComponent:** UI components available within the model panel. Different components are available (for example checkboxes, text fields and lists)

classes:

- *UIBooleanComponent*
- *UICompositionComponent*
- *UIConditionListComponent*
- *UIFloatComponent*
- *UIGeneralListComponent*
- *UIPhaseListComponent*
- *UITemperatureComponent*

1.3 Call Events for the Property Model Methods

The table lists which events trigger the property model methods (defined in the interface *PythonPropertyModel*):

| Interface method | Event triggering the method to be called |
|------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------|
| <code>before_evaluations()</code> | once after the Perform button is clicked, before any call to <code>evaluate_model()</code> |
| <code>evaluate_model()</code> | once for each set of conditions, always after the call to <code>before_evaluations()</code> |
| <code>get_thermocalc_system()</code> | before any other method call - if the system state in Thermo-Calc has changed |
| <code>provide_calculation_result_quantities()</code> | after each call to <code>evaluate_model()</code> |
| <code>provide_model_category()</code> | whenever the Thermo-Calc UI needs to (re-) display components containing model information (for example the model tree) |
| <code>provide_model_description()</code> | once when the model panel is painted (this happens also whenever a model gets checked in the model tree) |
| <code>provide_model_name()</code> | whenever the Thermo-Calc UI needs to (re-) display components containing model information (for example the model tree) |
| <code>provide_ui_panel_components()</code> | once when the model panel is displayed (this happens also whenever a model gets checked in the model tree) |

The methods of a single property model are always executed sequentially.

INSTALLING JYTHON AND SETTING UP AN IDE

2.1 Installing Jython

This section describes the installation of Jython 2.7.0, but you should install the latest available version.

Note: The Jython installation is only required if you want to have full support of your IDE during the model development (autocompletion, debugging, and so forth). The property models will run automatically in Thermo-Calc using the Jython installation already bundled to Thermo-Calc.

- Before installing Jython, you need to have a correctly working Java SDK installation as a prerequisite.
- Download the latest Jython distribution from www.jython.org (the current installer version is `jython-installer-2.7.0.jar`)
- Execute the installer JAR-file.
- Choose the *Standard* installation.

2.2 Setting up the IDE

The Python property models can be developed using any text editor. For full functionality (autocompletion, debugging, etc.) it is recommended to use a Python IDE. The options described are the *IDEs IntelliJ IDEA Ultimate* and *PyCharm Professional* developed by JetBrains. Another suitable example is the *Microsoft Visual Studio Community* using the *Python Tools for Visual Studio*. If **debugging** the property models is a requirement, then it is necessary to use **commercial** versions of *IntelliJ* or *PyCharm*, otherwise the *Community* editions are sufficient.

2.2.1 IntelliJ IDEA

The information in this section is applicable to IntelliJ IDEA 2016. It is primarily a Java IDE and requires a plugin for full support of Python:

- Go to **File -> Settings -> Plugins**.
- Choose **Search in repositories** to search for the *Python* plugin.
- Install the plugin.

Installing a *Python SDK*:

- Go to **File -> Project Structure**.
- Click the **+** to add a new SDK under **Platform Settings -> SDKs**.

- Choose **Python SDK** and **Add Local**.
- Select the file `jython.exe` within the Jython installation, typically located in `C:\jython2.7.0\bin\jython.exe`

Setting the *Project SDK* (required for each model):

- Choose the *Jython SDK* within the **Project** tab as your *Project SDK*.
- **Add a dependency to the Python property model API in the Modules tab:**
 - Choose your module and navigate to the **Dependencies** tab.
 - Click **+** and choose **JARs or directories ...**
 - Choose the Python property model API directory (`PropertyModels/Interface/ThermoCalcModelInterface` within the property model directory).

2.2.2 PyCharm

This is required for each model:

Installing a *Project Interpreter*:

- Go to **File -> Settings**.
- Add a new *Project Interpreter* by navigating to your project and clicking **+**.
- Choose **Add Local**.
- Select the file `jython.exe` within the Jython installation, typically located in `C:\jython2.7.0\bin\jython.exe`

Adding a dependency to the *Python property model API*:

- Click the settings button for the selected Jython interpreter within the *Project Interpreter* and choose **More ...**
- Choose the Jython interpreter in the list of available Python interpreters and click **Show paths for selected interpreters**.
- Click the **+** to add the Python property model API directory (`PropertyModels/Interface/ThermoCalcModelInterface` within the property model directory).

Note: When you add the Python property model API directory to the interpreter settings, it changes your Jython installation. Consequently you may want to use a virtual environment.

CREATING A NEW PROPERTY MODEL

A new property model can be created and modified at any time during a Thermo-Calc session. The model is automatically reloaded and you do not need to restart Thermo-Calc.

Note: All property models must be located in a subdirectory of the property model directory. It is located within the Thermo-Calc home directory, which differs for the supported platforms.

| Operating system | Property model directory |
|------------------|---------------------------------------------------------------------|
| Windows | C:\Users\Public\Public Documents\Thermo-Calc\ 2020a \PropertyModels |
| Linux | /home/user/Thermo-Calc/2020a/PropertyModels |
| Mac | /Users/Shared/Thermo-Calc/2020a/PropertyModels |

Make sure that the *Model directory* path in the Thermo-Calc dialog *Tools -> Options -> General* points to the correct property model directory path.

How to Create a New Model:

- Start Thermo-Calc.
- Add a Property Model Calculator to a project in Thermo-Calc.
- Create a new folder within the model directory (as per the installed location). The folder can be given any name.
- Create a new Python model file or copy a file from another model, such as a predefined one. The file extension is *.py. For now, ignore any error messages in the **Event Log** in Thermo-Calc stating that the file does not fulfill the requirements for a property model.
- Give the model a valid file name **identical to the model class name** (“XYModel.py”)
- Assign the Python interpreter and the dependency to the property model API within your IDE (see [Setting up the IDE](#))
- Extend the model class *XYModel* to fully implement the interface *PythonPropertyModel*
- Implement the model (see [Tutorial](#))

Thermo-Calc automatically updates the model whenever it is changed in an editor. If UI components are changed you need to reload the model. Do this by deselecting the check box next to the model and then selecting it again to reload the model.

The model directories can be moved and renamed during the Thermo-Calc session without limitation. When moving or deleting a model from a directory, it is required to move or delete the XYModel.py **and** the XYModel.py.encrypted file. If the encrypted file is left in its original place, that model will only be switched from the *debuggable* to the *non-debuggable* model (see [Debugging](#)).

Example models demonstrating the most important features can be found in the chapter [Tutorial](#) and in the property model directory.

Note: The Python file as well as the model class need to follow the syntax “XYModel”. **This name needs to be unique within all property models.** You can define other classes or methods within the model file as long as these do not interfere with the required syntax for a model.

Note: It is possible to store several models within one model directory. These are distinguished based on their model name.

TUTORIAL

4.1 Example 1: A Basic Property Model with Thermodynamic Properties

This tutorial demonstrates the most relevant tasks to create a property model. A basic property model is created that provides you with the fraction of a certain phase in dependency of any defined condition.

Let's first take a look at the complete model code. The source code **must** be saved in a file (e.g. `Example1Model.py`) in a subdirectory of the property model directory for your operating system (see *Creating a New Property Model* for details). You can copy the code below directly to your editor, but make sure to remove all line break characters.

```
from PythonPropertyModel import PythonPropertyModel
from ThermoCalcSystem import *
from ThermoCalcCalculator import ThermoCalcCalculator

class Example1Model(PythonPropertyModel):
    """Example 1"""
    _PHASE_FRACTION_QUANTITY = "PHASE_FRACTION_QUANTITY"
    _PHASE_LIST = "PHASE_LIST_COMPONENT"

    def __init__(self):
        """Constructor"""
        self._thermocalc_system = None # type: ThermoCalcSystem

    def get_thermocalc_system(self, thermocalc_system):
        """Called by Thermo-Calc whenever an updated state of the Thermo-Calc core_
        ↪system needs to be injected into the model"""
        self._thermocalc_system = thermocalc_system

    def before_evaluations(self, calculator):
        """Called by Thermo-Calc immediately before the first model evaluation (using_
        ↪evaluate_model). Use this method for any required preparations."""
        pass

    def provide_model_category(self):
        """Called by Thermo-Calc when the model should provide its category (shown in_
        ↪the Thermo-Calc model tree)."""
        return ["Examples"]

    def provide_model_name(self):
        """Called by Thermo-Calc when the model should provide its name (shown in the_
        ↪Thermo-Calc model tree)."""
        return "Example 1"
```

```
def provide_model_description(self, locale):
    """Called by Thermo-Calc when the model should provide its detailed_
↪description."""
    description = "This is an example model."
    return description

def provide_calculation_result_quantities(self):
    """Called by Thermo-Calc when the model should provide its result quantity_
↪objects."""
    result_quantities = [create_general_quantity(Example1Model._PHASE_FRACTION_
↪QUANTITY, "Phase fraction")]
    return result_quantities

def provide_ui_panel_components(self):
    """Called by Thermo-Calc when the model should provide its UI components for_
↪the model panel to be plotted."""
    ui_components = [create_phase_list_ui_component(Example1Model._PHASE_LIST,
↪"Phase: ", "Phase list", default_phase="FCC_A1")]
    return ui_components

def evaluate_model(self, calculator):
    """
    Called by Thermo-Calc when the model should be actually calculated.

    :param calculator:      Calculation engine
    :type calculator:       ThermoCalcCalculator
    """
    chosen_phase = self._thermocalc_system.get_ui_list_value(Example1Model._PHASE_
↪LIST)
    calculator.compute_equilibrium(True)
    phase_frac = calculator.get_single_value("NPM(" + chosen_phase + ")")
    self._thermocalc_system.set_result_quantity_value(Example1Model._PHASE_
↪FRACTION_QUANTITY, phase_frac)
```

Every property model is a Python model containing the model class. This class needs to be derived from `PythonPropertyModel`, which is the interface for all property models. You need to implement all of its abstract methods. Generally, when executing a property model, Thermo-Calc is calling these methods to either obtain information from the model or to transfer data to the model.

Note: The Python file as well as the model class must follow the syntax “XYModel”. **This name must be unique within all property models.** You can define other classes or methods within the model file as long as these do not interfere with the required syntax for a model.

4.1.1 Access to the Thermo-Calc System

At any time you can access all data from the Thermo-Calc system and especially from the predecessor activity nodes (for example from the System Definer) via a `ThermoCalcSystem` object. That object is updated when, for example, the configuration in the System Definer changes. If that happens, a new object is provided by Thermo-Calc to the model by calling `PythonPropertyModel.PythonPropertyModel.get_thermocalc_system()`. It is recommended that you define an instance variable, which gives access to the up-to-date object at all times:

```
def __init__(self):
    """Constructor"""
    self._thermocalc_system = None # type: ThermoCalcSystem

def get_thermocalc_system(self, thermocalc_system):
    """Called by Thermo-Calc whenever an updated state of the Thermo-Calc_
    ↪core system needs to be injected into the model"""
    self._thermocalc_system = thermocalc_system
```

Note: Any method within the API provides a docstring, that can be used by the IDE to provide you autocompletion and autodocumentation. But as Python is using duck-typing, the API cannot always derive the correct variable types automatically. The constructor above shows an example on how to give a type hint to the IDE (PyCharm / IntelliJ IDEA) to provide autocompletion (in the example for `self._thermocalc_system`).

4.1.2 Basic Information About the Model

These methods provide the model category, name and description and are used by Thermo-Calc to present the models within a tree component in the Property Model Calculator:

```
def provide_model_category(self):
    """Called by Thermo-Calc when the model should provide its category_
    ↪(shown in the Thermo-Calc model tree)."""
    return ["Examples"]

def provide_model_name(self):
    """Called by Thermo-Calc when the model should provide its name (shown_
    ↪in the Thermo-Calc model tree)."""
    return "Example 1"

def provide_model_description(self, locale):
    """Called by Thermo-Calc when the model should provide its detailed_
    ↪description."""
    description = "This is an example model."
    return description
```

A property model can be included in multiple categories. The description should contain helpful information to the user regarding the scientific background of the model as well a short description about how to use it. You can use usual string formatting (“\n”, ...)

4.1.3 Defining Input and Output Parameters

All required input parameters are defined by creating components for the User Interface (UI). Every output parameter is defined as a *ResultQuantity*.

```
def provide_calculation_result_quantities(self):
    """Called by Thermo-Calc when the model should provide its result_
    ↪quantity objects."""
    result_quantities = [create_general_quantity(Example1Model._PHASE_
    ↪FRACTION_QUANTITY, "Phase fraction")]
    return result_quantities
```

The result quantities need to be provided within a list. Several result quantity types are available that provide different predefined properties, for example for a temperature.

Caution: Every result quantity is expected to be provided in SI units.

The purpose of the result quantity objects is to provide a container for transferring calculation results from the model to Thermo-Calc for plotting and other tasks. You will later assign values to the result quantities in the `PythonPropertyModel.evaluate_model()` method.

```
def provide_ui_panel_components(self):
    """Called by Thermo-Calc when the model should provide its UI components,
    for the model panel to be plotted."""
    ui_components = [create_phase_list_ui_component(Example1Model._PHASE_
    LIST, "Phase: ", "Phase list", selected_phase="FCC_A1")]
    return ui_components
```

Each input parameter is represented by a UI-component. The property model API provides the most common ones. The order in the list defines the order of appearance in the Property Model Calculator window. You can later read the values set by the user in `PythonPropertyModel.evaluate_model()`.

Example of a more complex property model UI:

Liquidus and solidus temperature

| Configuration | Description |
|--------------------------------------|---------------------------------------------|
| Only calculate liquidus temperature: | <input type="checkbox"/> |
| Liquid phase: | LIQUID v |
| Upper temperature search limit: | 3000.0 |
| Max. number of iterations: | 10 |
| Global minimization for liquidus: | <input type="checkbox"/> |
| Global minimization for solidus: | <input checked="" type="checkbox"/> |

Calculation Type

☐ Single
 ☒ One axis
 ☐ Grid
 ☐ Min/Max
 ☐ Uncertainty

Grid Definitions

| Quantity | Min | Max | Number of steps |
|------------------------------------------------------|-----|-----|-----------------------------------------|
| Mass percent Cr v | 0.0 | 10 | 30 v |

4.1.4 Performing the Calculations

Any setup that is required before the calculations needs to be provided in the method `PythonPropertyModel.before_evaluations()`:

```
def before_evaluations(self, calculator):
    """Called by Thermo-Calc immediately before the first model evaluation,
    ↪ (using evaluate_model). Use this method for any required preparations."""
    pass
```

The model is evaluated separately for every set of conditions. This means that in case of varying, for example two component concentrations, the `PythonPropertyModel.evaluate_model()` method is called separately for each composition:

```
def evaluate_model(self, calculator):
    """
    Called by Thermo-Calc when the model should be actually calculated.

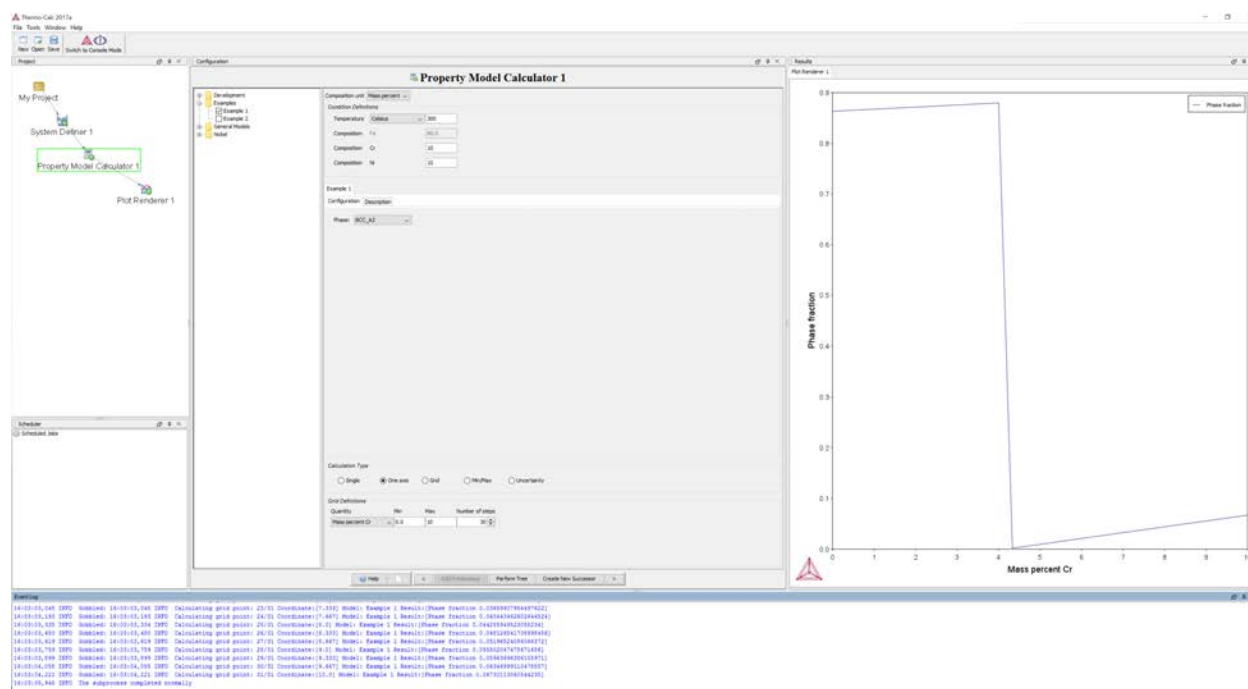
    :param calculator:      Calculation engine
    :type calculator:       ThermoCalcCalculator
    """
    chosen_phase = self._thermocalc_system.get_ui_list_value(Example1Model._
    ↪ PHASE_LIST)
    calculator.compute_equilibrium(True)
    phase_frac = calculator.get_single_value("NPM(" + chosen_phase + ")")
    self._thermocalc_system.set_result_quantity_value(Example1Model._PHASE_
    ↪ FRACTION_QUANTITY, phase_frac)
```

Note how type hinting for providing autocompletion is implemented in the example.

Tip: If sophisticated Thermo-Calc functionality is required that is not directly available within the Python API, Thermo-Calc Console Mode commands can be used: You have access to the full set of Thermo-Calc Console Mode commands available in Poly3 by using the methods `ThermoCalcCalculator.send_command_to_poly3()` and `ThermoCalcCalculator.get_single_value()`.

Caution: The lifetime of the `ThermoCalcCalculator` object is *restricted* to the subsequent calls to `PythonPropertyModel.evaluate_model()` and the initial `PythonPropertyModel.before_evaluations()` call while performing a model calculation. Consequently you must not store that object within an instance variable.

The screenshot shows an example calculation with the property model for the Fe - 10 Ni - x Cr system using the FEDEMO database, illustrating the functionality of the model:



4.2 Example 2: Property Model Using Apache Math

This example describes how to perform mathematical calculations using the Java Apache Math library. To keep it simple the sine of the temperature is calculated. This has limited practical application and is intended only as a demonstration.

Note: The Python property models in Thermo-Calc are executed as Jython code within the Java Virtual Machine of Thermo-Calc. It means that any Java library can be imported and used directly within the models. This includes the Apache Math library for numerical calculations.

Caution: Within Jython it is *not* possible to use any Python library based on native code (typically C-code). Consequently the property models **cannot use the numerical Python libraries NumPy and SciPy. Instead use the Java Apache Math library.**

The Apache Math library is automatically added to the classpath when executing the property model within Thermo-Calc. However, you will need to add a reference to the file `commons-math3-version.jar` in your IDE if you want to have autocompletion support. This file is located in the Thermo-Calc installation directory. For example IntelliJ IDEA supports referencing that Java-JAR, while this is not possible using PyCharm. However, this does not prevent you from running the property model in Thermo-Calc.

This is the code for the property model. Remember that it needs to be stored in the file `Example2Model.py` in a subdirectory of the property model directory:

```
# Python libraries
from PythonPropertyModel import PythonPropertyModel
from ThermoCalcCalculator import ThermoCalcCalculator
from ThermoCalcSystem import *
```

```

# Java libraries
from org.apache.commons.math3.analysis.function import Sqrt

class Example2Model(PythonPropertyModel):
    """Example 2"""
    _SQUARE_ROOT = "SQUARE_ROOT"
    _INVERT_RESULT_CHECKBOX = "INVERT_RESULT_CHECKBOX"

    def __init__(self):
        """Constructor"""
        self._thermocalc_system = None # type: ThermoCalcSystem
        self._sqrt_provider = Sqrt()

    def get_thermocalc_system(self, thermocalc_system):
        """Called by Thermo-Calc whenever an updated state of the Thermo-
        Calc core system needs to be injected
        into the model"""
        self._thermocalc_system = thermocalc_system

    def before_evaluations(self, calculator):
        """Called by Thermo-Calc immediately before the first model
        evaluation (using evaluate_model). Use this
        method for any required preparations."""
        pass

    def provide_model_category(self):
        """Called by Thermo-Calc when the model should provide its category
        (shown in the Thermo-Calc model tree)."""
        return ["Examples"]

    def provide_model_name(self):
        """Called by Thermo-Calc when the model should provide its name
        (shown in the Thermo-Calc model tree)."""
        return "Example 2"

    def provide_model_description(self, locale):
        """Called by Thermo-Calc when the model should provide its detailed
        description."""
        description = "This is an example model."
        return description

    def provide_calculation_result_quantities(self):
        """Called by Thermo-Calc when the model should provide its result
        quantity objects."""
        result_quantities = [create_general_quantity(Example2Model._SQUARE_
        ROOT, "Square root")]
        return result_quantities

    def provide_ui_panel_components(self):
        """Called by Thermo-Calc when the model should provide its UI
        components for the model panel to be plotted."""
        ui_components = [create_boolean_ui_component(Example2Model._INVERT_
        RESULT_CHECKBOX, "Invert result: ",
        "Determines if the result
        will be inverted ...", True)]
        return ui_components

```

```

def evaluate_model(self, calculator):
    """
    Called by Thermo-Calc when the model should be actually calculated.

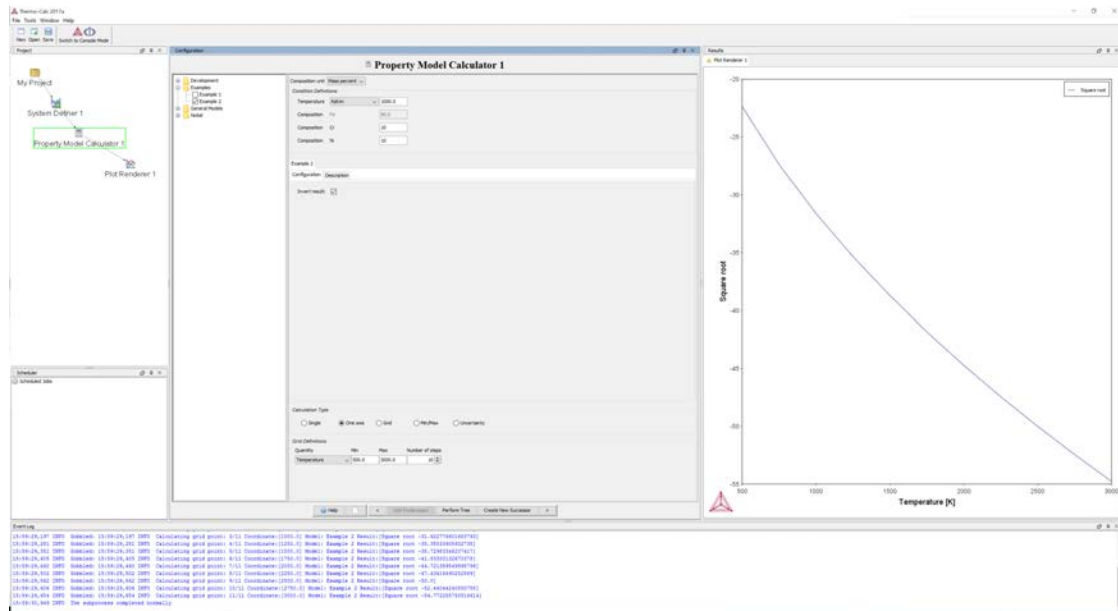
    :param calculator:      Calculation engine
    :type calculator:       ThermoCalcCalculator
    """
    temp = calculator.get_temperature()
    square_root = self._sqrt_provider.value(temp)
    if self._thermocalc_system.get_ui_boolean_value(Example2Model._
    ↪ INVERT_RESULT_CHECKBOX):
        square_root = -square_root

    self._thermocalc_system.set_result_quantity_value(Example2Model._
    ↪ SQUARE_ROOT, square_root)

```

In more practical examples, the numerical calculations would be coupled to thermodynamic calculations.

The screenshot shows an example of a calculation with the dummy property model:



DEBUGGING

All property models that are available as Python source code can be debugged from an IDE using a Python remote debugger.

Note: Most built-in Thermo-Calc property models are only available as encrypted files and cannot be debugged.

A property model is in the *debuggable* state, if its Python-file (`XYModel.py`) is available in the model directory in Thermo-Calc. If only the encrypted file (`XYModel.py.encrypted`) is present, it is in the *non-debuggable state* and can be executed but not debugged.

Remote debugging should be possible with any remote debugging library for Python that works with Jython. Thermo-Calc has tested *IntelliJ IDE Ultimate* / *PyCharm Professional* to work with the Thermo-Calc property models. You can use any editor or the Community edition of IntelliJ IDEA / PyCharm, however debugging of the models is not available.

5.1 Setting up IntelliJ IDEA / PyCharm for Debugging Models

It is expected that the IDE is set up completely according to *Setting up the IDE*.

The Thermo-Calc application is running in a Java Virtual Machine and is invoking the Python code of the model via Jython. The following steps are required to prepare remote debugging in IntelliJ IDEA Ultimate (note that the IntelliJ Community Edition does not provide remote debugging functionality):

- **Place the following lines in the Python model in front of the part you want to debug:**
 - Typically these are placed at the beginning of the `PythonPropertyModel.evaluate_model()` method:

```
import sys
sys.path.insert(0, "C:\\Users\\UserName\\.IntelliJ IDEA2016.
↳3\\config\\plugins\\python\\pycharm-debug.egg")
import pydevd
self._thermocalc_system.log_warning("Attach now to the process to proceed ...
↳") # optional to inform the user that the model waits for the debug server
pydevd.settrace('localhost', port=5678, stdoutToServer=True,
↳stderrToServer=True, suspend=True)
```

Warning:

- Currently you must not use the pydevd-library available via pip on PyPy. It is outdated and does not work as expected. Use the version bundled to IntelliJ IDEA as shown above.

- You may use any port; the only requirement is that it is unused by other programs.

- **Create a remote debugger configuration in IntelliJ:**

- Go to the menu “Run”, choose “Edit configurations” and add a configuration by clicking “+”.
- Choose “Python Remote Debug”.
- Give that configuration a good name, for example “Remote Debug Server”.
- Set the host name to “localhost” and the port to that defined in your Python source code (5678 in our example).

- **Start debugging:**

- Choose the remote debugging configuration defined above and start it in debug mode (*Ctrl + F9*). It should give now a wait message in the output window.
- Start your desired user-defined property model calculation in Thermo-Calc by clicking **Perform tree**. The model should now connect to the debug server and the IDE should stop directly after the `settrace()` call in the Python model.
- Now you can inspect your variables and step through the code. You can also use the “Debug Command Line” in the menu “Tools” for interactive testing.
- You can safely ignore warnings that are occurring.

Note: Thermo-Calc executes the model in a temporary subprocess. This means that the model opens a new connection to the debug server during each execution. This is intended behavior and implies that the connection does not need to be closed manually.

5.2 Editing Your Model during a Thermo-Calc Session

You can edit your model at any time, once it is saved. It is **automatically reloaded** by Thermo-Calc and can immediately be used without restarting Thermo-Calc. You can also debug the edited model.

Note: If IntelliJ IDEA misses a source file during remote debugging, it opens an empty file `<string>` or emits error messages similar to “Error in file “`<string>`”, line unknown” if the source file where the error occurred cannot be found. In that case you can still proceed debugging by using “Resume Program” (using the *F9* key).

Warning: Thermo-Calc does not trigger reloading the model if another imported module than the model itself has been edited.

PROVIDING TRANSLATIONS

The Property Model Framework supports multi-language property models based on Java Properties-files. All property models released by Thermo-Calc are using that mechanism to provide a user interface in all languages supported by Thermo-Calc. This functionality can be as well applied by any user in their own property models.

6.1 Example

The following code snippet shows how to implement localized property models using the class *JavaPropertyManager* (the model needs to have the source file name `MyModel.py`):

```
from JavaPropertyManager import JavaPropertyManager
# further imports to come here

def __init__(self):
    """Constructor"""
    self._properties = JavaPropertyManager("MyModel")

# all other methods to come here

def provide_model_name(self):
    """Called by Thermo-Calc when the model should provide its name (shown in the_
    ↪ Thermo-Calc model tree)."""
    return self._properties.get("modelName.text")
```

The corresponding snippet of the Properties-file `MyModel.properties` could look like that:

```
modelName.text=MyModel
modelCategory.text=General Models
```

For example a Properties-file `MyModel_de.properties` that is translated to German looks like:

```
modelName.text=Mein Modell
modelCategory.text=Allgemein
```

6.2 Java Properties-files

The class *JavaPropertyManager* automatically chooses the language that is currently set in Thermo-Calc. When using localization, you need to provide at least the default Properties-file (syntax: `XYModel.properties`). In that file the English translations should be provided. Further translations can be provided in Properties-files with the syntax

`XYModel_sv.properties` (or equivalent for other languages). If the required Properties-file or a certain key is missing, Thermo-Calc uses automatically the key in the default Properties-file.

The Properties-files must either be placed in the property model resources directory `jythonModelsResources` that is located in the program file directory of your installation (for example `C:\Program Files\Thermo-Calc\ 2020a\jythonModelsResources` on Windows) or you can pass a user-defined location to the *JavaPropertyManager* constructor.

Please obtain more general information on Java Properties-files from the Java documentation if required.

API REFERENCE

7.1 PythonPropertyModel Interface

class PythonPropertyModel.**PythonPropertyModel**

Bases: org.python.proxies.PythonPropertyModel\$PythonPropertyModel\$14

Customer-available Python property model API interface. The model object is created once ahead of each calculation (in its own subprocess) after the user clicks “Perform”.

before_evaluations (*calculator*)

Called by Thermo-Calc immediately before the first model evaluation (using `evaluate_model`). Use this method for any required preparations.

Parameters **calculator** (*ThermoCalcCalculator*) – calculation engine, this object exists only during this method call and the following `evaluate_model()` call and will be destroyed afterwards. Therefore do not store this object outside of the method.

evaluate_model (*calculator*)

Called by Thermo-Calc when the model should be actually calculated.

Parameters **calculator** (*ThermoCalcCalculator*) – calculation engine, this object exists only during this method call and the previous `before_evaluations()` call and will be destroyed afterwards. Therefore do not store this object outside of the method. The object contains all required information from the Thermo-Calc core for the calculation.

get_thermocalc_system (*thermocalc_system*)

Called by Thermo-Calc whenever an updated state of the Thermo-Calc core system needs to be injected into the model. Thread-safety is guaranteed, i.e. the method will only be called directly before but never during other API method calls.

Parameters **thermocalc_system** (*ThermoCalcSystem*) – Thermo-Calc core system providing access to all information on the thermodynamic system currently defined by the user. This object is guaranteed to live until it is replaced. It can and should be stored in an instance variable within the model class.

provide_calculation_result_quantities ()

Called by Thermo-Calc when the model should provide its result quantity objects.

Returns result quantity objects of the model (to be filled later with results in `evaluate_model()`)

Return type list of ResultQuantity

provide_model_category ()

Called by Thermo-Calc when the model should provide its category (shown in the Thermo-Calc model tree).

Returns category of the model, it may be present in several categories

Return type list of str

provide_model_description (*locale*)

Called by Thermo-Calc when the model should provide its detailed description.

Parameters **locale** (*java.util.Locale*) – locale of the model provided for a localized (language-dependent) description

Returns description text for the model

Return type str

Raises **RuntimeException** – if the model requires a locale, it should throw if the locale is not provided

provide_model_name ()

Called by Thermo-Calc when the model should provide its name (shown in the Thermo-Calc model tree).

Returns name of the model

Return type str

provide_model_parameters ()

Called by Thermo-Calc when the model should provide all model parameters and their current values. **Optional.**

Note: These are internal variables of the property model that are intended to be modified from the outside. Typically this is used to adjust their values in a optimizer during the development of the model.

Returns the model parameter ids and their current values

Return type dict(str, float) [unit according to the parameter meaning]

provide_ui_panel_components ()

Called by Thermo-Calc when the model should provide its UI components for the model panel to be plotted.

Returns model UI panel components in the order to be presented in the model panel

Return type list of UIComponent

set_model_parameter (*model_parameter_id, value*)

Called by Thermo-Calc when a model parameter should be reset. **Optional.**

Note: These are internal variables of the property model that are intended to be modified from the outside. Typically this is used to adjust their values in a optimizer during the development of the model.

Parameters

- **model_parameter_id** – The parameter id
- **value** – The value [unit according to the parameter meaning]

7.2 ResultQuantity

class ResultQuantity.**ResultQuantity** (*quantity_id, description, quantity_type*)

Defines a calculation result quantity of a property model that is identified by a unique ID

Constructor.

Parameters

- **quantity_id**(*str*) – unique ID of the quantity
- **description**(*str*) – description of the quantity (shown in the Thermo-Calc UI)
- **quantity_type**("enum" defined in *ResultQuantity*) – type of the quantity (defines the unit)

ENERGY_QUANTITY = 2

GENERAL_QUANTITY = 0

STRENGTH_QUANTITY = 3

TEMPERATURE_QUANTITY = 1

TIME_QUANTITY = 4

get_description()

Obtains the description of the quantity.

Returns description of the quantity

Return type str

get_id()

Obtains the ID of the quantity.

Returns unique ID of the quantity

Return type str

get_type()

Obtains the type of quantity.

Returns type of the quantity

Return type "enum" defined in *ResultQuantity*

7.3 ThermoCalcCalculator

class ThermoCalcCalculator.PhaseStatus

Bases: object

Defines the status of a phase

DORMANT = 2

ENTERED = 0

FIXED = 1

SUSPENDED = 3

class ThermoCalcCalculator.SearchDirection

Bases: object

Defines the search direction in the compute_transition() method

NEGATIVE = 0

POSITIVE = 1

class ThermoCalcCalculator.**ThermoCalcCalculator** (*model_engine*)

Bases: object

Thermodynamic calculation engine of Thermo-Calc for the property models

Constructor. Note: This class should never be instantiated by the model, it will always be provided by Thermo-Calc with the correct and updated data.

Parameters *model_engine* (*se.thermocalc.externalapi.propertymodel.ModelEngine*) – Thermo-Calc internal property model engine

compute_chemical_diffusion_coefficient (*phase*, *diffusing_constituent*, *gradient_constituent*, *reference_constituent*)

Computes a chemical diffusion coefficient.

Parameters

- **phase** (*str*) – name of the phase of interest
- **diffusing_constituent** (*str*) – name of the diffusing constituent
- **gradient_constituent** (*str*) – name of the gradient constituent
- **reference_constituent** (*str*) – name of the reference constituent

Returns the chemical diffusion coefficient (in m/s^2)

Return type float

compute_equilibrium (*use_global*)

Performs a thermodynamic equilibrium calculation using the current settings of the calculator

Parameters *use_global* (*bool*) – flag defining if global minimization is used: true for using it, false for not using it

compute_intrinsic_diffusion_coefficient (*phase*, *diffusing_constituent*, *gradient_constituent*, *reference_constituent*)

Computes an intrinsic diffusion coefficient.

Parameters

- **phase** (*str*) – name of the phase of interest
- **diffusing_constituent** (*str*) – name of the diffusing constituent
- **gradient_constituent** (*str*) – name of the gradient constituent
- **reference_constituent** (*str*) – name of the reference constituent

Returns the intrinsic diffusion coefficient (in m/s^2)

Return type float

compute_tracer_diffusion_coefficient (*phase*, *constituent*)

Computes a tracer diffusion coefficient.

Parameters

- **phase** (*str*) – name of the phase of interest
- **constituent** (*str*) – name of the diffusing constituent

Returns the chemical diffusion coefficient (in m/s^2)

Return type float

compute_transition (*phase_to_form*, *condition_to_relax*, *step_length*, *direction*, *use_global*)

Compute transition command identical to that of the Thermo-Calc console. Determines the occurrence of a phase transition when varying a certain condition. Example: solvus temperature of a phase. Note: After finishing, this command has adjusted the equilibrium present in the calculator to the requested transition. The requested properties such as the transition temperature can be read using the appropriate methods.

Parameters

- **phase_to_form** (*str*) – name of the phase to be formed
- **condition_to_relax** (*str*) – condition to be relaxed in Thermo-Calc console syntax (e.g. “T” or “W(CR)”)
- **step_length** (*float*) – step length of the relaxed condition, the minimum possible value is 1.0, the unit is that of the condition
- **direction** (*SearchDirection*) – direction of search for the relaxed condition (positive or negative)
- **use_global** (*bool*) – flag defining if global optimization is used

delete_condition (*condition_in_classic_syntax*)

Deletes a condition from the calculator.

Parameters **condition_in_classic_syntax** (*str*) – condition to be deleted in Thermo-Calc console syntax

get_conditions ()

Obtains the currently defined conditions in the calculator.

Returns list of conditions currently defined in the calculator in Thermo-Calc console syntax

Return type list of str

get_degrees_of_freedom ()

Obtains the degrees of freedom in current calculator.

Returns degrees of freedom in the current calculator

Return type int

get_molar_volume (*phase_name*)

Obtains the molar volume of a phase.

Parameters **phase_name** (*str*) – name of the phase

Returns the molar volume of that phase

Return type float

get_phase_status (*phase_name*)

Obtains the current status of a phase.

Parameters **phase_name** (*str*) – name of the phase

Returns status of that phase

Return type *PhaseStatus*

get_single_value (*command_in_classic_syntax*)

Obtains any single value from the calculator using the Thermo-Calc console syntax. Can be used as a workaround for commands not existing in the property model API.

Parameters **command_in_classic_syntax** (*str*) – Thermo-Calc console syntax command specifying the value

Returns the requested value in the same unit as it would be in the Thermo-Calc console mode

Return type float

get_stable_phases_in_equilibrium()

Obtains all phases there are stable in the current equilibrium.

Returns all phases stable in the current equilibrium

Return type list of str

get_temperature()

Obtains the currently set temperature in the calculator.

Returns the currently set temperature (in K)

Return type float

send_command_to_poly3(*command_in_classic_syntax*)

Sends a console syntax command directly to the Poly3 model. This command accepts all console commands available in POLY3 and can be used as a workaround for commands not existing in the property model API.

Parameters **command_in_classic_syntax** (*str*) – Thermo-Calc console syntax command

set_component_entered(*component*)

Sets a component to status ENTERED in the calculator.

Parameters **component** (*str*) – name of the component

set_component_special(*component*)

Sets a component to status SPECIAL in the calculator.

Parameters **component** (*str*) – name of the component

set_component_suspended(*component*)

Sets a component to status SUSPENDED in the calculator.

Parameters **component** (*str*) – name of the component

set_condition(*condition_in_classic_syntax*)

Sets a new condition in the calculator.

Parameters **condition_in_classic_syntax** (*str*) – new condition in Thermo-Calc console syntax

set_phase_dormant(*phase*)

Sets a phase to the status DORMANT.

Parameters **phase** (*str*) – name of the phase to be set to the status dormant

set_phase_entered(*phase, amount*)

Sets a phase to the status ENTERED.

Parameters

- **phase** (*str*) – name of the phase to be set to the status entered
- **amount** (*float*) – phase fraction amount of that phase ($0.0 < \text{amount} < 1.0$)

set_phase_fixed(*phase, amount*)

Sets a phase to the status FIXED.

Parameters

- **phase** (*str*) – name of the phase to be set to the status FIXED

- **amount** (*float*) – phase fraction amount of that phase ($0.0 < \text{amount} < 1.0$)

set_phase_suspended (*phase*)

Sets a phase to the status SUSPENDED.

Parameters **phase** (*str*) – name of the phase to be set to the status SUSPENDED

set_temperature (*temp*)

Sets the temperature in the calculator.

Parameters **temp** (*float*) – new temperature (in K)

suspend_all_phases ()

Sets all phases in the present calculator to the status SUSPENDED.

7.4 ThermoCalcSystem

class ThermoCalcSystem.SpecialListMarkers

Bases: object

Placeholders for special list elements that are locale-dependent. They will be provided by UI list components if a special marker has been selected.

ANY_LIST_MARKER = u'ANY'

NONE_LIST_MARKER = u'NONE'

class ThermoCalcSystem.ThermoCalcSystem (*model_utils*)

Provides all helper functionality required within the property models to access the Thermo-Calc / GUI functionality

Constructor. Note: This class should never be instantiated by the model, it will always be provided by Thermo-Calc with the correct and updated data.

Parameters **model_utils** (*se.thermocalc.externalapi.propertymodel.ModelUtils*) – Internal model utils object from the Thermo-Calc property model core

get_components ()

Obtains all components currently set in the system.

Returns all defined components :rtype: list of str

get_dependent_component ()

Obtains the currently set dependent component of the system, i.e. that component that is typically the main element of an alloy, for example Fe or Ni.

Returns the dependent component

Return type str

get_non_dependent_components ()

Obtains the currently set non-dependent components of the system, i.e. all components except the dependent “main” component.

Returns the non-dependent components

Return type list of str

get_object_from_previous_evaluation (*key*)

Retrieves a stored object from a previous evaluation.

Parameters **key** (*str*) – key of the object

Returns the stored object

Return type object

get_selected_phases ()

Obtains all currently selected phases in the system.

Returns the names of all selected phases

Return type list of str

get_ui_boolean_value (*component_id*)

Obtains the value from the specified checkbox.

Parameters **component_id** (*str*) – ID of the checkbox

Returns setting of the checkbox

Return type bool

get_ui_composition_value (*component_id*)

Obtains the composition from the specified composition UI component.

Parameters **component_id** (*str*) – ID of the composition UI component

Returns composition (in mole or mass fraction), note that the input unit of the UI is specified in the model panel. If required, the composition is automatically converted to fractions.

Return type float

get_ui_double_value (*component_id*)

Obtains the value from the specified UI component.

Parameters **component_id** (*str*) – ID of the UI component

Returns value

Return type float

get_ui_list_value (*component_id*)

Obtains the selected entry from a UI component list. If a special element (such as ANY, NONE, ...) is selected, the corresponding locale-independent placeholder is provided.

Parameters **component_id** (*str*) – ID of the list UI component

Returns selected entry

Return type str

get_ui_temperature_value (*component_id*)

Obtains the temperature from the specified temperature UI component.

Parameters **component_id** (*str*) – ID of the temperature UI component

Returns temperature (in K), note that input unit of the UI is specified in the model panel. If required, the temperature is automatically converted to K.

Return type float

is_object_saved (*key*)

Determines if an object is stored for the specified key.

Parameters **key** (*str*) – object key

Returns true if an object has been saved for the specified key, false otherwise.

Return type bool

is_phase_gas (*phase_name*)

Determines if a phase is a gas phase.

Parameters **phase_name** (*str*) – name of the phase

Returns true if the phase is a gas phase, false otherwise

Return type bool

is_phase_liquid (*phase_name*)

Determines if a phase is a liquid phase.

Parameters **phase_name** (*str*) – name of the phase

Returns true if the phase is a liquid phase, false otherwise

Return type bool

log_debug (*s*, **arg*)

Logs a debug level message to the Thermo-Calc log message window. Example:
self._thermocalc_system.log_debug("Phase {} is invalid", phase_name)

Parameters

- **s** (*str*) – log message
- **arg** (*any*) – string arguments, can be omitted

log_error (*s*, **arg*)

Logs an error level message to the Thermo-Calc log message window. Example:
self._thermocalc_system.log_error("Phase {} is invalid", phase_name)

Parameters

- **s** (*str*) – log message
- **arg** (*any*) – string arguments, can be omitted

log_info (*s*, **arg*)

Logs an info level message to the Thermo-Calc log message window. Example:
self._thermocalc_system.log_info("Phase {} is invalid", phase_name)

Parameters

- **s** (*str*) – log message
- **arg** (*any*) – string arguments, can be omitted

log_trace (*s*, **arg*)

Logs a trace level message to the Thermo-Calc log message window. Example:
self._thermocalc_system.log_trace("Phase {} is invalid", phase_name)

Parameters

- **s** (*str*) – log message
- **arg** (*any*) – string arguments, can be omitted

log_warning (*s*, **arg*)

Logs a warning level message to the Thermo-Calc log message window. Example:
self._thermocalc_system.log_debug("Phase {} is invalid", phase_name)

Parameters

- **s** (*str*) – log message
- **arg** (*any*) – string arguments, can be omitted

num_saved_objects()

Determines the number of objects stored between evaluations.

Returns number of objects stored

Return type int

save_object_for_next_evaluation(*key*, *object_to_be_saved*)

Stores any object between evaluations and make it available for the next evaluation. This allows to overcome the limited lifetime of the ThermoCalcCalculator object.

Parameters

- **key** (*str*) – key of the object for later access
- **object_to_be_saved** (*object*) – object to be stored

set_result_quantity_value(*quantity_id*, *value*)

Sets the value of a previously defined result quantity for further usage in the Thermo-Calc property model core for plotting, ...

Parameters

- **quantity_id** (*str*) – unique ID of the result quantity
- **value** (*float*) – value to be set (use float('NaN') in case of an invalid result)

ThermoCalcSystem.**create_boolean_ui_component**(*component_id*, *name*, *description*, *initial_setting*)

Creates a UI checkbox component for a boolean value. The value of that component can later be accessed during the model evaluation.

Parameters

- **component_id** (*str*) – unique ID of the component
- **name** (*str*) – name of the component, will be presented in the model panel
- **description** (*str*) – additional description of the component
- **initial_setting** (*bool*) – initial setting of the checkbox

Returns the created component

Return type *UIBooleanComponent*

ThermoCalcSystem.**create_composition_ui_component**(*component_id*, *name*, *description*, *initial_composition*)

Creates a UI text field component for a composition value. The value of that component can later be accessed during the model evaluation.

Parameters

- **component_id** (*str*) – unique ID of the component
- **name** (*str*) – name of the component, will be presented in the model panel
- **description** (*str*) – additional description of the component
- **initial_composition** (*float*) – initial composition to be set in the text field (unit defined by the user in the Thermo-Calc system)

Returns the created component

Return type *UICompositionComponent*

ThermoCalcSystem.**create_condition_list_ui_component** (*component_id, name, description*)

Creates a UI list component for all conditions defined in the system. The value of that component can later be accessed during the model evaluation.

Parameters

- **component_id** (*str*) – unique ID of the component
- **name** (*str*) – name of the component, will be presented in the model panel
- **description** (*str*) – additional description of the component

Returns the created component

Return type *UIConditionListComponent*

ThermoCalcSystem.**create_energy_quantity** (*quantity_id, description*)

Creates a energy result quantity (in J). When the model is evaluated, a value can be added to the quantity and it will be used to transfer the result to the Thermo-Calc plot engine.

Parameters

- **quantity_id** (*str*) – unique ID of the result quantity
- **description** (*str*) – additional description of the result quantity

Returns the created result quantity

Return type *ResultQuantity*

ThermoCalcSystem.**create_float_ui_component** (*component_id, name, description, value*)

Creates a UI text field component for a real number. The value of that component can later be accessed during the model evaluation.

Parameters

- **component_id** (*str*) – unique ID of the component
- **name** (*str*) – name of the component, will be presented in the model panel
- **description** (*str*) – additional description of the component
- **value** (*float*) – initial setting of the text field

Returns the created component

Return type *UIFloatComponent*

ThermoCalcSystem.**create_general_quantity** (*quantity_id, description*)

Creates a general result quantity that can contain any type of result (without a unit). When the model is evaluated, a value can be added to the quantity and it will be used to transfer the result to the Thermo-Calc plot engine.

Parameters

- **quantity_id** (*str*) – unique ID of the result quantity
- **description** (*str*) – additional description of the result quantity

Returns the created result quantity

Return type *ResultQuantity*

ThermoCalcSystem.**create_list_ui_component** (*component_id, name, description, entry_list, selected_entry=""*)

Creates a UI list component for string entries. The value of that component can later be accessed during the model evaluation.

Parameters

- **component_id** (*str*) – unique ID of the component
- **name** (*str*) – name of the component, will be presented in the model panel
- **description** (*str*) – additional description of the component
- **entry_list** (*list of str*) – entries of the list
- **selected_entry** (*str*) – entry to be initially selected. If omitted, by default the first element is selected.

Returns the created component

Return type *UIGeneralListComponent*

ThermoCalcSystem.**create_phase_list_ui_component** (*component_id, name, description, default_phase="", any_marker=False*)

Creates a UI list component for all phases defined in the system. It is possible to select a default phase that is supposed to be the **expected phase selection** for that list. The value of that component can later be accessed during the model evaluation.

A **default** phase is the phase that is initially selected and re-selected as soon as a currently selected phase is removed. If the default phase is not available, a NONE-marker will be created and used instead of the default phase. A typical use case for the default phase setting is a phase list that expects to contain the LIQUID-phase of a system.

Parameters

- **component_id** (*str*) – unique ID of the component
- **name** (*str*) – name of the component, will be presented in the model panel
- **description** (*str*) – additional description of the component
- **default_phase** (*str*) – default phase, if omitted no default phase is chosen and only initially the first element of the list is selected. If an ANY-marker is added, this is chosen as the default element.
- **any_marker** (*bool*) – defines if an entry “ANY PHASE” should be added to the phase list, if set to true this overrides any default phase setting

Returns the created component

Return type *UIPhaseListComponent*

ThermoCalcSystem.**create_strength_quantity** (*quantity_id, description*)

Creates a strength result quantity (in MPa). When the model is evaluated, a value can be added to the quantity and it will be used to transfer the result to the Thermo-Calc plot engine.

Parameters

- **quantity_id** (*str*) – unique ID of the result quantity
- **description** (*str*) – additional description of the result quantity

Returns the created result quantity

Return type *ResultQuantity*

ThermoCalcSystem.**create_temperature_quantity** (*quantity_id, description*)

Creates a temperature result quantity (in K). When the model is evaluated, a value can be added to the quantity and it will be used to transfer the result to the Thermo-Calc plot engine.

Parameters

- **quantity_id** (*str*) – unique ID of the result quantity
- **description** (*str*) – additional description of the result quantity

Returns the created result quantity

Return type *ResultQuantity*

ThermoCalcSystem.**create_temperature_ui_component** (*component_id*, *name*, *description*,
initial_temp)

Creates a UI text field component for a temperature value. The value of that component can later be accessed during the model evaluation.

Parameters

- **component_id** (*str*) – unique ID of the component
- **name** (*str*) – name of the component, will be presented in the model panel
- **description** (*str*) – additional description of the component
- **initial_temp** (*float*) – initial temperature to be set in the text field (unit defined by the user in the Thermo-Calc system)

Returns the created component

Return type *UITemperatureComponent*

ThermoCalcSystem.**create_time_quantity** (*quantity_id*, *description*)

Creates a time result quantity (in s). When the model is evaluated, a value can be added to the quantity and it will be used to transfer the result to the Thermo-Calc plot engine.

Parameters

- **quantity_id** (*str*) – unique ID of the result quantity
- **description** (*str*) – additional description of the result quantity

Returns the created result quantity

Return type *ResultQuantity*

7.5 UIBooleanComponent

class UIBooleanComponent.**UIBooleanComponent** (*component_id*, *name*, *description*, *setting*)

Bases: *UIComponent*.*UIComponent*

Checkbox UI component of the model panel

Constructor.

Parameters

- **component_id** (*str*) – unique ID of the component
- **name** (*str*) – name of the component, will be presented in the model panel
- **description** (*str*) – additional description of the component
- **setting** (*bool*) – initial setting of the checkbox

connect_component_visibility (*dependent_component_id*)

Connects the visibility of any other UI component of the model panel to the value of the check box.

Parameters `dependent_component_id (str)` – ID of the UI element to be dependent on the chosen element

get_dependent_components ()

Obtains a list containing all UI elements currently connected regarding their visibility.

Returns a list of all all UI elements currently connected

get_setting ()

Obtains the initial setting of the checkbox.

Returns initial setting of the checkbox

Return type bool

remove_component_visibility (dependent_component_id)

Removes the visibility connection to a UI component that has been previously connected.

Parameters `dependent_component_id (str)` – ID of the previously connection UI element

7.6 UIComponent

class `UIComponent.UIComponent (component_id, name, description)`

Bases: object

Base class for all UI components of the model panel

Constructor.

Parameters

- **component_id (str)** – unique ID of the component
- **name (str)** – name of the component, will be presented in the model panel
- **description (str)** – additional description of the component

get_description ()

Obtains the additional description of the component.

Type additional description of the component

Return type str

get_id ()

Obtains the unique ID of the component.

Returns unique ID of the component

Return type str

get_name ()

Obtains the name of the component.

Type name of the component, will be presented in the model panel

Return type str

7.7 UICompositionComponent

class UICompositionComponent.**UICompositionComponent** (*component_id, name, description, composition*)

Bases: *UIComponent.UIComponent*

Composition text field UI component of the model panel

Constructor.

Parameters

- **component_id** (*str*) – unique ID of the component
- **name** (*str*) – name of the component, will be presented in the model panel
- **description** (*str*) – additional description of the component
- **composition** (*float*) – initial composition to be set in the text field (unit defined by the user in the Thermo-Calc system)

get_composition ()

Obtains the initial composition set in the text field in the UI.

Returns initial composition to be set in the text field (unit defined by the user in the Thermo-Calc system)

Return type float

7.8 UIConditionListComponent

class UIConditionListComponent.**UIConditionListComponent** (*component_id, name, description*)

Bases: *UIComponent.UIComponent*

System condition list UI component of the model panel

Constructor. All conditions are set automatically.

Parameters

- **component_id** (*str*) – unique ID of the component
- **name** (*str*) – name of the component, will be presented in the model panel
- **description** (*str*) – additional description of the component

7.9 UIFloatComponent

class UIFloatComponent.**UIFloatComponent** (*component_id, name, description, value*)

Bases: *UIComponent.UIComponent*

General real value text field UI component of the model panel

Constructor.

Parameters

- **component_id** (*str*) – unique ID of the component
- **name** (*str*) – name of the component, will be presented in the model panel

- **description** (*str*) – additional description of the component
- **value** (*float*) – initial setting of the text field

get_value ()

Obtains the initial setting of the text field.

Returns initial setting of the text field

7.10 UIGeneralListComponent

class UIGeneralListComponent.**UIGeneralListComponent** (*component_id, name, description, content, selected_entry*="")

Bases: *UIComponent.UIComponent*

General list UI component of the model panel that can contain any strings

Constructor.

Parameters

- **component_id** (*str*) – unique ID of the component
- **name** (*str*) – name of the component, will be presented in the model panel
- **description** (*str*) – additional description of the component
- **content** (*list of tuple of str*) – entries of the list, they need to contain a locale-independent ID and a localized content string, for example: [("ENTRY_1_ID", "entry 1"), (ENTRY_2_ID, "entry 2")]
- **selected_entry** (*str*) – entry to be initially selected. If omitted, by default the first element is selected.

connect_component_visibility (*dependent_component_id, selected_item_to_set_visible*)

Connects the visibility of any other UI component of the model panel to the selection of a certain entry of the list.

Parameters

- **dependent_component_id** (*str*) – ID of the UI element to be dependent on the chosen element
- **selected_item_to_set_visible** (*str*) – entry (locale independent ID) of the list to be chosen to set the dependent component visible

get_content ()

Obtains the entries of the list.

Returns entries of the list, they need to contain a locale-independent ID and a localized content string, for example: [("ENTRY_1_ID", "entry 1"), (ENTRY_2_ID, "entry 2")]

Return type list of tuple of str

get_dependent_components ()

Obtains a dictionary containing all UI elements currently connected regarding their visibility.

Returns all UI elements currently connected (key: dependent component ID, value: required list entry to set it visible)

Return type dict(str, str)

get_selected_entry()

Obtains the initially selected entry.

Returns initially selected entry. If empty, the first element is selected.

Return type str

remove_component_visibility(*dependent_component_id*)

Removes the visibility connection to a UI component that has been previously connected.

Parameters **dependent_component_id** (*str*) – ID of the previously connection UI element

7.11 UIPhaseListComponent

```
class UIPhaseListComponent.UIPhaseListComponent(component_id, name, description, default_phase="", any_marker_setting=False)
```

Bases: *UIComponent.UIComponent*

Phase list UI component of the model panel

Constructor.

Parameters

- **component_id** (*str*) – unique ID of the component
- **name** (*str*) – name of the component, will be presented in the model panel
- **description** (*str*) – additional description of the component
- **default_phase** (*str*) – default phase, if omitted no default phase is chosen and only initially the first element of the list is selected. If an ANY-marker is added, this is chosen as the default element.
- **any_marker_setting** (*bool*) – defines if an entry “ANY PHASE” should be added to the phase list, if set to true this overrides any default phase setting

get_any_marker_setting()

Obtains the setting if any entry “ANY PHASE” is added to the phase list.

Returns if an entry “ANY PHASE” is added to the phase list, if set to true this overrides any default phase setting

Return type bool

get_default_phase()

Obtains the default phase.

Returns default phase, if omitted no default phase is chosen and only initially the first element of the list is selected. If an ANY-marker is added, this is chosen as the default element.

Return type str

7.12 UITemperatureComponent

```
class UITemperatureComponent.UITemperatureComponent(component_id, name, description, temp)
```

Bases: *UIComponent.UIComponent*

Temperature value text field UI component of the model panel

Constructor.

Parameters

- **component_id** (*str*) – unique ID of the component
- **name** (*str*) – name of the component, will be presented in the model panel
- **description** (*str*) – additional description of the component
- **temp** (*float*) – initial temperature to be set in the text field (unit defined by the user in the Thermo-Calc system)

get_temp ()

Obtains the initial temperature set in the text field.

Returns initial temperature to be set in the text field (unit defined by the user in the Thermo-Calc system)

Return type float

7.13 JavaPropertyManager

class `JavaPropertyManager.JavaPropertyManager` (*class_name*, *resource_dir_path=None*)

Bases: `object`

Providing localized strings based on Java property file bundles.

Constructor. It is expected that Java **.properties* files of the format “*class_name_sv.properties*” are provided. A default file with the name “*class_name.properties*” containing the english strings is required.

Parameters

- **class_name** (*str*) – name of the Python class for which the properties need to be provided
- **resource_dir_path** (*str*) – path to directory containing the resource file, if omitted the resources are expected to be located in the subdirectory `RESOURCES_DIR` of the Thermo-Calc program directory

`JAVA_PROPERTY_EXTENSION = '.properties'`

`RESOURCES_DIR = 'jythonModelsResources'`

get (*property_key*)

Obtains a property for the class specified in the constructor.

Parameters **property_key** (*str*) – property key (for example “*label.text*”, ...)

Returns localized string

Return type str

Thermo-Calc User Guide: Console Mode

Thermo-Calc Version 2020a



Working in Console Mode

In this section:

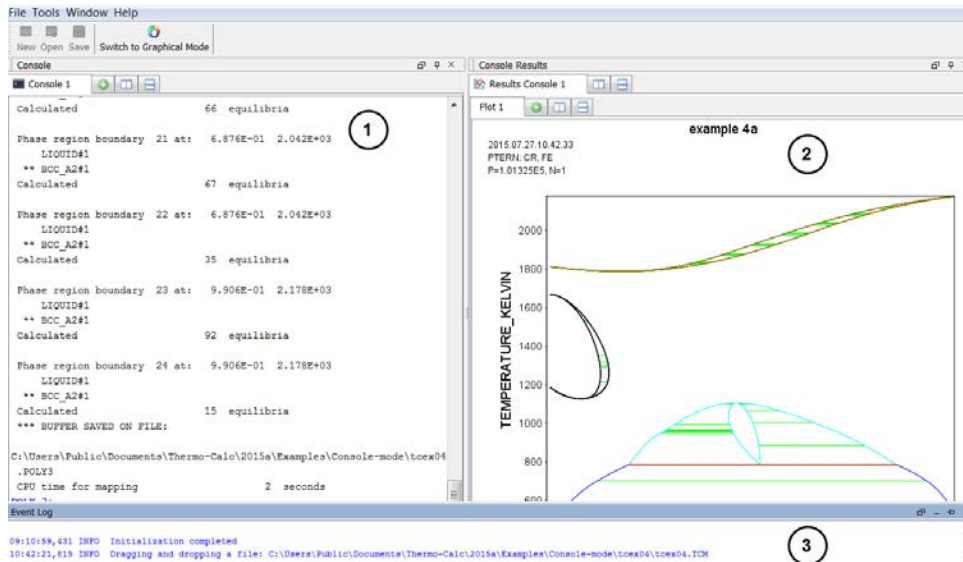
| | |
|---------------------------------------------------|---|
| The Console Mode Layout | 2 |
| Console Window | 3 |
| Console Mode Results Window | 4 |
| Event Log Window | 4 |
| Keyboard Shortcuts to Navigate Between Tabs | 4 |

The Console Mode Layout

By default the first time you launch Thermo-Calc it opens in Graphical Mode. After this, the mode defaults to the most recent one. You can switch back and forth between modes. To open the Console Mode interface, click **Switch to Console Mode** on the toolbar.

▶ ["Keyboard Shortcuts to Navigate Between Tabs" on page 4](#)

THE CONSOLE MODE USER INTERFACE

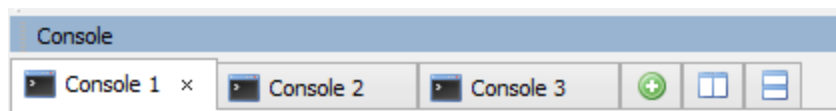





The currently selected window is called the *active* window. This has a darker title bar than the other windows. The windows are:

1. **Console**, with a **Console 1** tab.
2. **Console Results**, with a **Results Console 1** tab as well as a sub-tab (**Plot 1**), which is what is displayed in the window in the figure.
3. **Event Log**, which is the active window in this example.

CONSOLE TABS

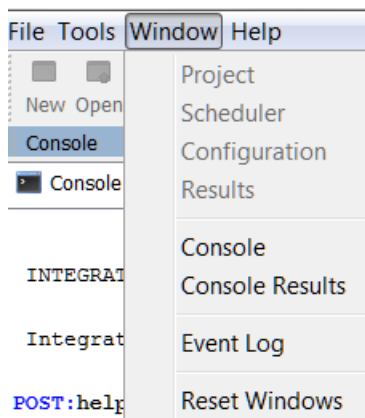
By default, the tabs are side-by-side:



You can toggle to view the tabs top-to-bottom/stacked (click the  button) and back to side-by-side (click the  button) or the  button.

OPEN CONSOLE WINDOWS



Open a specific window from the **Window** main menu, or select **Reset Windows** to return to the default window layout.



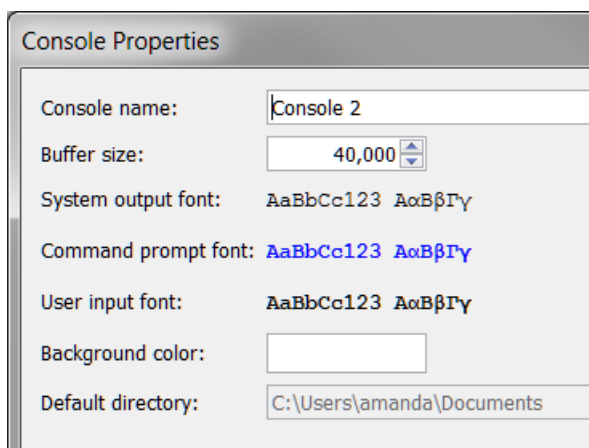
Console Window

By default the Console window is on the left-hand side of the console. This is where you enter commands. The window can have several Console tabs.

To open and close Console tabs:


- To open (or add), click the  button, press <Ctrl+T> when the Console window is active, or right-click a tab header and select **New Console**.
- To close, click the  button, press <Ctrl+W> or <Ctrl+F4>, or right-click the tab header and select **Close**.
- To close all tabs except one, right-click the header of the tab you want to keep and select **Close Other**.
- To close all tabs and open a new one, right-click the header of any tab and select **Close All**.

You can change the tab name, font and colors for an individual Console tab by right-clicking its header and selecting **Properties**.



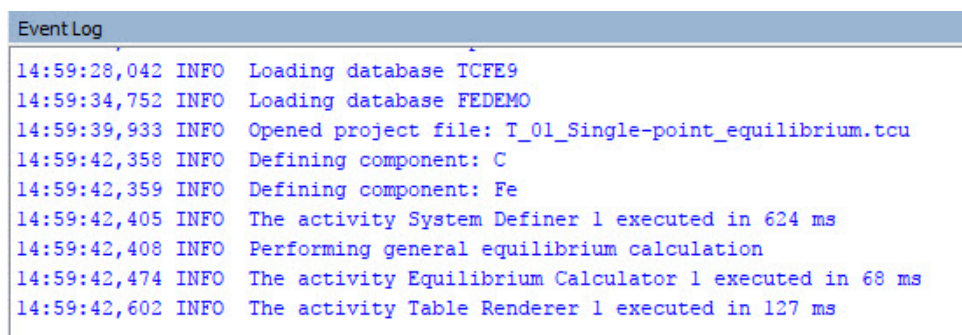
Console Mode Results Window

By default, the Console Results window is on the right-hand side of the screen. This is where plotted diagrams display. Each Console has its own Results tab in the Results window. All the plots and tables generated are presented in the Results tab.

- To open new **Plot** tabs press <Ctrl+Shift+T> or click the add  button.
- To open a new Plot tab for the currently active Console tab, press <Ctrl+Shift+T>. To close the Plot tab, press <Ctrl+Shift+W> or <Ctrl+Shift+F4>.

Event Log Window

By default the Event Log window is collapsed (closed). It includes important information about the commands that run and are completed, including error messages. Click once to toggle it open and closed.



Keyboard Shortcuts to Navigate Between Tabs

Use keyboard shortcuts to move between the tabs available in the Console and Results windows.

WINDOWS

- Press CTRL + TAB to move forward sequentially through each open tab. When you are focused on the Console window, you move forward simultaneously through the Console Results tabs, e.g. If you are on Console 1 and press CTRL + TAB, you move forward to Console 2 and Results Console 2 and so forth.

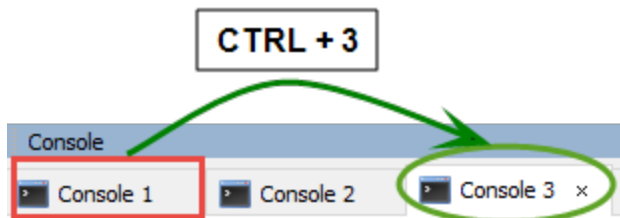


- Press CTRL + SHIFT + TAB to move back through the open tabs. This is useful if you have multiple tabs open, otherwise you can use the CTRL + TAB to cycle through the windows.
- Press CTRL + [tab number 1 to 9] to move directly to the numbered tab. For example, if you are focused on Console 1 and want to move to Console 3, press CTRL+3 and the focus jumps to that tab.



The tab number corresponds to the order of the tabs, not necessarily the name. That is, if Console 4 is first, then it is what is highlighted when CTRL + 1 is used.

For **EXAMPLE**, press CTRL + 3 on the keyboard to move focus from Console 1 to Console 3.



When you are focused on the **Console Results** window and use any of the shortcuts this only moves you through the open tabs on this window.

LINUX AND MAC

The same **Windows** keyboard shortcuts are used but must be pressed twice to move forward and backward.

Modules and Commands

In this section:

| | |
|-----------------------------------------------|----|
| Console Mode Workflow | 7 |
| Defining a System in Console Mode | 8 |
| Console Mode Modules | 9 |
| Moving Between Modules and Submodules | 13 |
| Entering Command Names or Abbreviations | 14 |
| Using the Command Line Prompt | 15 |
| Main Menu Commands | 15 |
| Command History | 16 |
| Wild Card Characters | 17 |

Console Mode Workflow

Working with Thermo-Calc involves moving between different modules. The workflow differs depending on the type of calculation:

- If you want to perform a calculation using the **POLY** module, you typically first retrieve thermodynamic data in the **DATA** module, perform the calculation in **POLY**, and visualize the results in the **POST** module. It is possible to define a system directly in **POLY** using the **DEFINE_MATERIAL** and **DEFINE_DIAGRAM** commands.
- If you want to calculate and plot a diagram using a response-driven module, such as **POTENTIAL** or **SCHEIL**, then you can go directly to that module. Response-driven modules prompt you to go through the steps to do the calculation and the required post-processing. These modules include **BIN**, **TERN**, **POTENTIAL**, **POURBAIX**, and **SCHEIL**. You typically end up in the **POST** module after having used a response-driven module. In the **POST** module you can modify the plots and save the diagram.
- If you want to tabulate a chemical substance, phase, or reaction, go directly to the **TAB** module.

The basic workflow is:

1. You are in the **SYS** module when you start Thermo-Calc in Console Mode.
2. In the **DATA** module define the system. Before performing a calculation, you must define the system and retrieve thermodynamic data. The data is retrieved from a database file (*.TDB or *.TDC).
3. The data needed to describe a system is then sent to the **GIBBS** module. This data is accessed by the **POLY** module when you instruct it to perform calculations.
4. In the **POLY** module, perform the calculations.
 - In **POLY**, the conditions are set for an equilibrium calculation (temperature, pressure, system composition, etc.), then an equilibrium calculation is done.
 - If you want to make a property or phase diagram, you set the conditions for a stepping or mapping operation and perform that operation.
 - This generates data that can be used to plot a property diagram (if a stepping operation is performed) or a phase diagram (if a mapping operation is performed).
5. In the **POST** module plot and visualize your data.
 - If a stepping or mapping operation is performed, then you can go to the **POST** module and plot a property or phase diagram.

-
- The diagram can be plotted quickly using default settings, but you can also modify which variables to plot of the diagram axes and change the appearance of the diagram.
 - You can save the diagram either as a plain text file with data about all the coordinates or as an image file.

Defining a System in Console Mode

Defining a system means to select the chemical components and to retrieve thermodynamic data about those components from an appropriate database in order to do the calculations. You use database(s) with thermodynamic data and then define what system elements as components. Once the system is defined, you retrieve the system's thermodynamic data from the database(s).

- If you use a *response-driven module* to perform your calculation, such as BIN or POURBAIX, then the module prompts you to select database(s) and define the system.
- When doing calculations in the POLY module, you typically have to manually select databases and define the system in the DATA module. However, it is also possible to define the system directly in POLY using the DEFINE_MATERIAL and DEFINE_DIAGRAM commands.

▶ ["Database \(TDB\) Module Commands" on page 122](#)

HOW TO DEFINE A SYSTEM IN CONSOLE MODE

1. Go to the DATA (TDB) module. At the `SYS` prompt, use `GOTO_MODULE` and enter `Data`.
2. Change the default database unless you directly specify the name of the database as a parameter to the command. Type `SWITCH_DATABASE` and follow the prompts.

The second part of the command prompt indicates the current default database. For example, if the prompt is `TDB_TCFE9`, then the current database is TCFE9.

3. Use `DEFINE_ELEMENTS` followed by a list of the elements that you want in your system. (To list the elements that are available in your current database, use `LIST_DATABASE` and choose `Elements`). For example, if you want to have Fe and C in your system, type:

```
DEFINE_ELEMENTS Fe C
```

-
4. Use REJECT and choose `Phases` if you want to avoid retrieving any phases from the database. (To list the phases that are available in your current database, use LIST_DATABASE and choose `Phases`. To list the phases that can form in the defined system, use LIST_SYSTEM and choose `Constituent`.) For example, if you do not want the graphite phase to be retrieved, you type:

```
REJECT PHASES GRAPHITE
```

If the number of phases to include is much lower than the total number of phases, then it can be convenient to first `Reject Phases *` and then restore the phases to include using `Restore Phases`.

5. Use GET_DATA to search the database and send the thermodynamic data about your system to the GIBBS workspace.

At this point you can proceed to the POLY module (with GOTO_MODULE POLY). However, you may want to add elements, phases and species to the GIBBS workspace from other databases. If so, then proceed to the next step.

6. Use APPEND_DATABASE to select the (additional) database from which you want to retrieve data. This command works exactly in the same way as the SWITCH_DATABASE command, with the exception that it does not reinitialize the DATA module and the GIBBS workspace, but instead appends or replaces the data that has already been retrieved with new data from the additional database.
7. Define your elements and specify whether to reject and restore any phases. Do this in exactly the same way when using the SWITCH_DATABASE command (see steps 2 and 3).
8. Use GET_DATA to search the database and add the thermodynamic data to the data that already exists in the GIBBS workspace.
9. Use APPEND_DATABASE again if you want to add data from yet another database. When you have retrieved all the data you need, you can proceed to the POLY module.

Console Mode Modules

▶ ["Graphical Mode Activities vs Console Mode Modules " on page 7](#)

Below are each of the available modules you access in Console Mode. Most of the modules have commands, some are the same no matter what module you are in (e.g. general commands like BACK, GO TO MODULE, EXIT, HELP and so forth). Other commands have different prompts based on the module you are in how you define the system and so forth.



Most modules have several commands available. The exceptions are the BINARY, TERNARY, SCHEIL, POURBAIX and POTENTIAL modules which do not have any additional commands once you access the modules. These are response-driven modules that prompt you with a series of questions and then build the diagram automatically based on your responses.

SYSTEM UTILITIES (SYS)

This is the module where you start. It also has several commands. Throughout the other modules there are some general commands, both of which are listed together.

▶ ["System Utilities \(SYS\) Commands" on page 111](#)

GIBBS ENERGY SYSTEM (GES)

The Gibbs Energy System (GES) module is an important Thermo-Calc Console Mode module and consists of a comprehensive subroutine package for various thermochemical calculations. The module is interactively connected with all basic and advanced modules in Thermo-Calc and the add-on Diffusion Module (DICTRA). Most users will not directly use the GES module and commands unless you perform assessments.



The GES module is in essence the Thermo-Calc calculation engine, sometimes referred to as the *calculation core*. When working in Graphical Mode you are using the GES calculation engine behind the scenes, whereas in Console Mode, and if you are performing assessments, you are directly interacting with the module. This is also applicable if you are working with any of the software development kits (SDKs).

▶ ["About the Gibbs Energy System \(GES\) Module" on page 36](#)

▶ ["Gibbs Energy System \(GES\) Commands" on page 202](#)

POLY3 (POLY) (EQUILIBRIUM)

With the equilibrium calculation module, POLY3, it is possible to calculate many different kinds of equilibria and diagrams, in particular multicomponent phase diagrams.

▶ ["The Equilibrium Calculation Module \(POLY3\)" on page 39](#)

-
- ▶ ["POLY Module Commands" on page 131](#)

DATABASE (TDB)

The Database module (full name is Database Retrieval) is where you select and retrieve various types of thermodynamic and kinetic information from the selected databases you are going to use for your system. Once you enter the module the short name is `TDB`.

- ▶ ["Database \(TDB\) Module Commands" on page 122](#)
- ▶ ["Defining a System in Console Mode" on page 8](#)
- ▶ Also see the ["Database Manager User Guide" on page 1](#) and the available information for the specific databases.

POST - A POLY3 SUBMODULE

The POST module (post-processor) is a submodule to the POLY module and has its own set of commands. The TAB, BIN, TERN, POT, SCHEIL and POURBAIX modules use the POST module features as part of the automatic generation of the plots.

- ▶ ["Using the POST Module" on page 101](#)
- ▶ ["POST Module Commands" on page 350](#)

SCHEIL (SCHEIL) SIMULATIONS

The variants of the Scheil-Gulliver solidification simulation (classic Scheil simulation, Scheil with a fast diffuser element, and Scheil with back diffusion) are set up in either the SCHEIL module in Console Mode or the Scheil Calculator in Graphical Mode.



The Scheil with back diffusion feature is only available for systems with diffusion data, i.e. it requires the use of a mobility database.

The Scheil calculation allows the calculation of:

- The solidification range of an alloy.
- Depression of the solidus temperature due to segregation.
- Composition of the last liquid to disappear in segregation pockets.

-
- Phases formed on final solidification in segregation pockets.
 - The composition gradient in the primary solid phase(s) (segregation profile).

▶ ["About the Scheil-Gulliver Solidification Simulations " on page 72](#)

▶ ["SCHEIL Module Commands" on page 246](#)

POURBAIX DIAGRAM (POURBAIX)

The POURBAIX module lets you construct Pourbaix diagrams and other types of property diagrams for heterogeneous interaction systems with aqueous solution phases. Once you have calculated the Pourbaix diagram, you can also use the saved results of the calculation (the POLY3-file), and make a property diagram based on stepping calculation. You can also plot additional diagrams based on the results of the same calculation, but with different axis variables than Ph and Eh.

▶ ["About Aqueous Solutions and the Pourbaix Diagram" on page 82](#)

POTENTIAL DIAGRAM (POT)

The POTENTIAL_DIAGRAM module (short name, the POTENTIAL module) is a potential phase diagram calculation module. A potential diagram uses the activities of two major species in the gaseous mixture phase as mapping variables.

▶ ["About Potential Diagrams" on page 67](#)

BINARY DIAGRAM (BIN)

The BINARY_DIAGRAM module (short name, the BIN module) enables you to quickly calculate a simple binary phase diagram. Binary phase diagrams are by far the most common found in the literature and calculated by computers. However, most real systems have more than two components and thus binary diagrams are more a kind of exercise in order to calculate more realistic phase diagrams.

▶ ["About Binary Phase Diagrams" on page 53](#)

TERNARY DIAGRAM (TERN)

The TERNARY_DIAGRAM module (short name, the TERN module) enables you to quickly calculate a simple ternary phase diagram. There are many types of ternary phase diagrams

but perhaps the most common is the isothermal section. In this case, the temperature is constant, which means that the tie-lines are in the plane of the calculation.

▶ ["About Ternary Phase Diagrams" on page 54](#)

PARROT (OPTIMIZATION)

The PARROT module makes use of the GES module to handle the models of the various phases that might form in a multicomponent system, as well as of the POLY module to store and calculate complex heterogeneous equilibria.

▶ ["PARROT Module Commands" on page 255](#)

▶ Also see the ["Data Optimization User Guide" on page 1](#)

TABULATION REACTION (TAB)

The TABULATION_REACTION (TAB) module can be used to tabulate thermodynamic functions of any type of substance, stoichiometric phase or solution phase, or reaction. The module can tabulate thermodynamic functions of pure stoichiometric phases or solution phases at fixed composition, as well as various kinds of partial derivatives for a pure stoichiometric phase or solution phase at a given composition.

▶ ["About the Tabulation Reaction Module" on page 95](#)

▶ ["Tabulation Reaction \(TAB\) Commands" on page 321](#)

REACTOR SIMULATOR (REACTOR)

Simulate chemical reaction processes in several feed-forward steady-state stages or in several dynamic stages.

▶ ["REACTOR \(REACTOR_SIMULATOR\) Commands" on page 342](#)

DICTRA MONITOR (DICTRA)

DICTRA Monitor (DICTRA) and DIC Parrot (optimization for DICTRA): These are available with the add-on Diffusion Module.

Moving Between Modules and Submodules

To go to a specific module, you typically use GOTO_MODULE (or just GOTO) followed by the name of the module. For example, to go to the DATA module, type `GOTO DATA`.

The exceptions are the submodules POST and ED-EXP:

- To go to the POST module, you must enter the POST command from within the POLY module or DICTRA module (if you have the add-on license).
- To go to the Edit Experiments module you must enter the ED-EXP command from within the PARROT module.

To go back to the previous module type `Back`. For example, if you are in the DATA module and entered it from the SYS module, when you type `Back`, you return to the SYS prompt. This command is also available to exit from the submodules POST and ED-EXP.



Without a valid Thermo-Calc license, you cannot leave the SYS module. To enter the DICTRA and DIC_PARROT modules, you also need a valid Diffusion Module (DICTRA) license key.

Entering Command Names or Abbreviations

The name of a command typically consists of terms linked with underscores, for example, LIST_EQUILIBRIUM. Note the following:

- UPPER or lower case letters are OK.
- Hyphens (-) instead of underscores (_) are OK, e.g. LIST-EQUILIBRIUM.
- You can abbreviate commands as long as it is unambiguous, e.g. when more than one command begins with LIST_, you need to type the next letter or word to distinguish between the commands.
- Each word can be abbreviated e.g., L_E for LIST_EQUILIBRIUM.

EXAMPLES

These are examples of how you can abbreviate commands at the command line prompt.

| Command name | Abbreviation |
|--------------------------|--------------|
| CALCULATE_EQUILIBRIUM | C-E |
| CALCULATE_ALL_EQUILIBRIA | C-A |
| LIST_EQUILIBRIUM | L-E |
| LIST_INITIAL_EQUILIBRIUM | LI-I-E |
| LOAD_INITIAL_EQUILIBRIUM | LO-I-E |
| LIST_PHASE_DATA CBCC | L-P-D CBC |

| Command name | Abbreviation |
|--------------------------------------------|----------------------------|
| LIST_PHASE_DATA CEMENTITE | L-P-D CEM |
| SET_ALL_START_VALUES | S-A-SS-AL |
| SET_AXIS_VARIABLE 1 X(FCC,FE) 0 0.89 0.025 | S-A-V 1 X(F,FE) 0 .89 .025 |
| SET_START_CONSTITUENT | S-S-C |
| SET_START_VALUE | S-S-V |
| SET_AXIS_PLOT_STATUS | S-A-P |
| SET_AXIS_TEXT_STATUS | S-A-T-SS-A-TE |
| SET_AXIS_TYPE | S-A-TY |
| SET_OPTIMIZING_CONDITION | S-O-C |
| SET_OPTIMIZING_VARIABLE | S-O-V |
| SET_OUTPUT_LEVEL | S-O-LS-OU |

Using the Command Line Prompt

The command line prompt in the Console window tells you which module you are currently in. When Thermo-Calc is first opened in Console Mode, you are in the SYS module, which is indicated with the command line prompt `SYS`.

To use Console Mode, you type in commands at the command line prompt. The available commands depend on which module you are in. You can list the commands by typing `?` at the prompt and then press <Enter>.

- ["Moving Between Modules and Submodules" on page 13](#)
- ["Entering Command Names or Abbreviations" on the previous page](#)
- ["Specifying Parameters" on page 379](#)
- ["Wild Card Characters" on page 17](#)
- ["Command History" on the next page](#)
- ["Keyboard Shortcuts to Navigate Between Tabs" on page 4](#)
- ["Working with the Console Mode Output " on page 108](#)

Main Menu Commands



In Console Mode you use commands to access these menu options. If there is an equivalent command, it is listed below.



The **File** menu and toolbar are reserved for Graphical Mode. The **Tools**, **Window** and **Help** menus are described in ["Menu, Toolbar and Keyboard Shortcuts" on page 4](#).

OPEN FILES

- In the SYS module: ["MACRO_FILE_OPEN" on page 114](#)
- In the SYS module: ["OPEN_FILE" on page 117](#)

► ["Opening Console Mode Macro Files" on page 20](#)



Drag and drop files into the Console window to open or run a macro, for example. File types that can be opened this way are macro files (*.TCM and *.DCM), database files (*.TDB), and workspace files (*.POLY3, *.GES5, *.PAR, and *.DIC). Note that *.DCM and *.DIC file extensions are applicable to the Diffusion Module (DICTRA). Note that GES6 workspace files cannot yet be dragged and dropped.

SAVE (WORKSPACE)

This command depends on the module you are in. Type ? at the prompt to look for a command such as ["SAVE_GES_WORKSPACE" on page 243](#) (GIBBS module).

EXIT

In any module: EXIT

CLOSE

In the SYS module: ["CLOSE_FILE" on page 112](#)

DISPLAY LICENSE INFO

In the SYS module: ["DISPLAY_LICENSE_INFO" on page 112](#)

Command History

- To scroll through the last twenty commands used, type two exclamation marks (!!) and press <Enter>.

- To repeat the last n commands, type ! followed by the number of previous commands to be executed again.
- To scroll through previous performed commands, use the Up (↑) or Down arrow (↓) keys.
- To read more information about the command history functionality in Thermo-Calc, type ! ? at the command line prompt.

Wild Card Characters

You can sometimes use the asterisk (*) as a wild card character to, for example, refer to all components, phases, or species, when showing calculated properties in the POLY module, or when you set axis variables for plotting diagrams in the POST module.

When showing calculated properties in the POLY module, you can also use the dollar sign (\$) to refer to all stable phases.



For activity and/or chemical potential properties, the * and \$ normally do not work properly as wild card characters.

EXAMPLES

These are examples of the wild card characters you can use to search commands at the command line prompt.

| Command | Action |
|-------------------------|----------------------------------------------------------------------|
| SHOW_VALUE B(*) | Lists mass (gram) of all components in the system. |
| SET_AXIS_VAR Y B(*) * | Sets mass (gram) of all components in the system as Y-axis variable. |
| SHOW_VALUE MUR(*) | Lists chemical potentials of all components in the system. |
| SET_AXIS_VAR Y ACR(*) * | Sets activities of all components in the system as Y-axis variable. |
| SHOW_VALUE HM(*).T | Lists heat capacities of all phases. |
| SET_AXIS_VAR Y GM(*) * | Sets molar Gibbs free energies of all phases as Y-axis variable. |
| SHOW_VALUE TC(\$) | Lists curie temperature of all stable phases. |
| SHOW_VALUE W(*,*) | Lists mass fractions of all components in all phases. |
| SHOW_VALUE W(\$,*) | Lists mass fractions of all components in all stable phases. |

| Command | Action |
|---------------------|------------------------------------------------------------------------------|
| SHOW_VALUE W(FCC,*) | Lists mass fractions of all components in the FCC phase. |
| SHOW_VALUE W(*,FE) | Lists mass fractions of the Fe component in all phases. |
| SHOW_VALUE W(\$,FE) | Lists mass fractions of the Fe component in all stable phases. |
| SHOW_VALUE Y(*,*) | Lists site fractions of all species in all sublattices of all phases. |
| SHOW_VALUE Y(\$,*) | Lists site fractions of all species in all sublattices of all stable phases. |
| SHOW_VALUE Y(*,*) | Lists site fractions of all species in all sublattices of all phases. |

File Types

In this section:

| | |
|------------------------------------------------|----|
| Working with the Console Mode File Types | 20 |
| Opening Console Mode Macro Files | 20 |
| Log Files | 23 |
| Macro Files | 24 |
| Workspace Files | 26 |
| Editing the Default Console Directory | 29 |
| Experimental Data Files (*.POP, *.DOP) | 31 |

Working with the Console Mode File Types



For DICTRA Console Mode see *File Formats* in the *Diffusion Module (DICTRA) User Guide*

In Console Mode, Thermo-Calc uses different types of files, including:

- ["Macro Files" on page 24](#) and ["Log Files" on page 23](#) both with the file extension *.TCM. Log files are created using the SET_LOG_FILE command.
- ["Workspace Files" on page 26](#) in POLY (*.POLY3), GIBBS module (*.GES5), and the PARROT module (*.PAR). (For the GIBBS module, this cannot currently be done with GES6).
- ["Experimental Data Files \(*.POP, *.DOP\)" on page 31](#) are a type of workspace file available with the PARROT module and have the file extension of *.POP. In the Diffusion Module (DICTRA), you work with .DOP files instead of .POP. These .POP and .DOP files are referred to as experimental data files.



Another type of experimental data file with the *.EXP file extension are also generated when working with DATAPLOT. See ["About the DATAPLOT Graphical Language" on page 3](#).



A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.



Drag and drop files into the Console window to open or run a macro, for example. File types that can be opened this way are macro files (*.TCM and *.DCM), database files (*.TDB), and workspace files (*.POLY3, *.GES5, *.PAR, and *.DIC). Note that *.DCM and *.DIC file extensions are applicable to the Diffusion Module (DICTRA). Note that GES6 workspace files cannot yet be dragged and dropped.

Opening Console Mode Macro Files



The macro files (with the extension *.TCM) include comments, which you can either run in Thermo-Calc or open and read in a text editor.

You can open the macro files (*.TCM or *.DCM files) in different ways.

-
- From the main menu,
 - Using a command,
 - By dragging and dropping the file into the Console window, or
 - Navigate to the file location on your computer and double-click to open it. If you already have Thermo-Calc open, this opens a new instance of the software.
 - You can also read the commands listed in the macro file using a text editor.



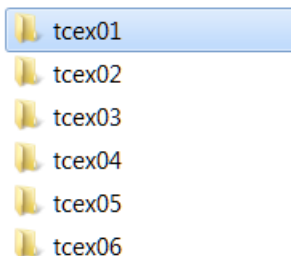
If you only open and read the macro file in a text editor, you do not see the output that Thermo-Calc gives in response to the commands stored in the macro file.

Opening a Macro from the Main Menu

To open an example macro file for Thermo-Calc:

1. Open Thermo-Calc.
2. Confirm you are in Console Mode. If not, click the **Switch to Console Mode** button.
3. From the main menu, select **File →** or **Help → Examples Files**. The Console Mode folder opens.
4. Open the **Thermo-Calc** folder to see the available examples contained in separate folders.

Name



For the Diffusion Module (DICTRA) examples (*.DCM macro files), open the **Diffusion Module - DICTRA** folder.

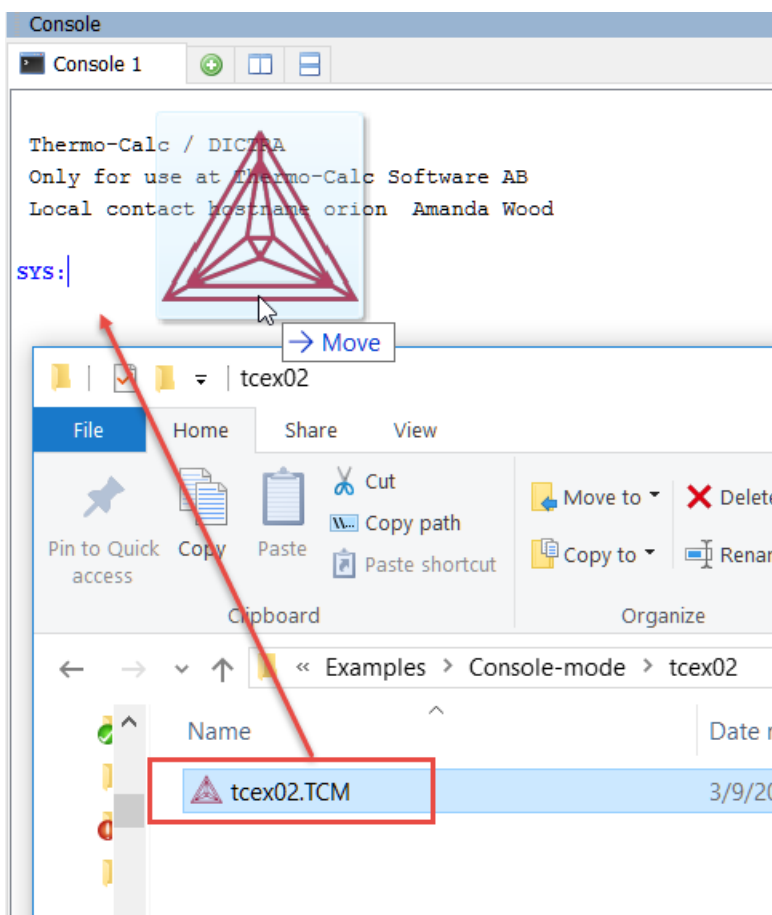
5. In the folder, double-click the *.TCM file or click **Open**.
6. Follow the prompts in the Console window i.e. keep pressing <Enter> to run the macro and produce a plot in the **Console Results** window.

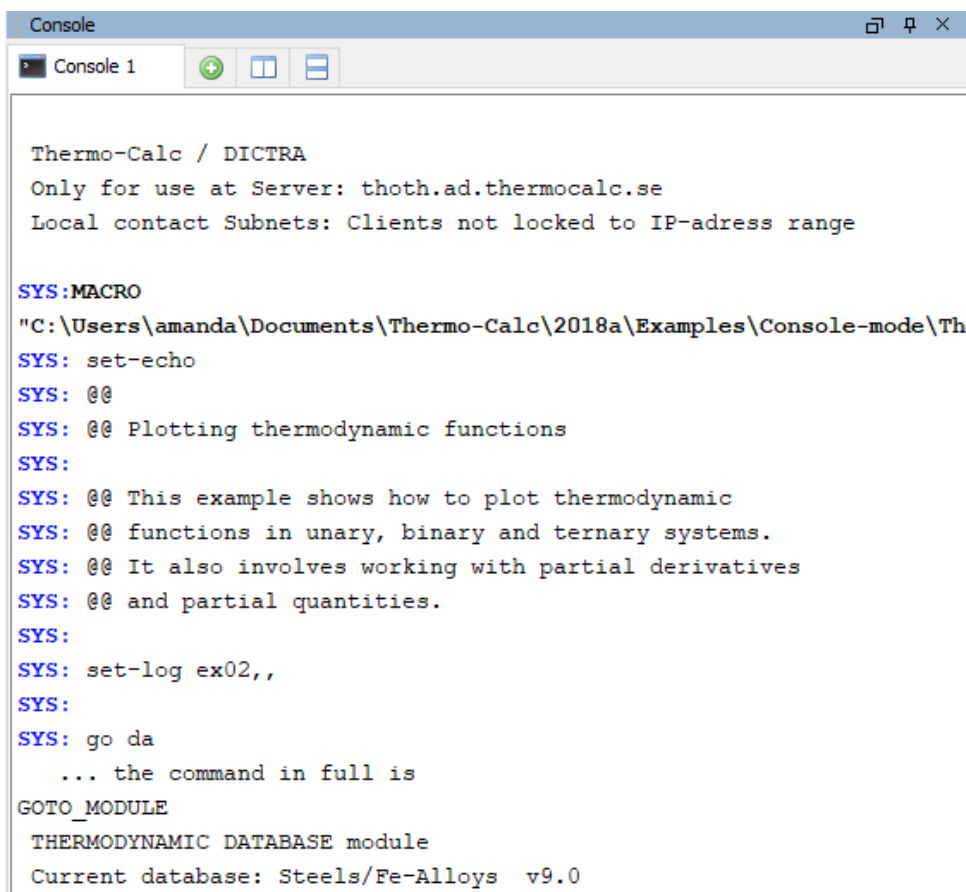
Opening a Macro Using a Command

At the `sys` prompt, type `MACRO_FILE_OPEN` and press <Enter>. In the file dialogue window that opens, navigate to and select the macro file to open.

Drag and Drop a Macro File into the Console Window

For example, on your computer, navigate to the examples folder. Drag the file from its location into the Thermo-Calc Console window. When you release (drop) the file, the macro starts running. Follow the prompts in the Console window i.e. keep pressing <Enter> to run the macro and produce a plot in the **Console Results** window.





```
Thermo-Calc / DICTRA
Only for use at Server: thoth.ad.thermocalc.se
Local contact Subnets: Clients not locked to IP-address range

SYS:MACRO
"C:\Users\amanda\Documents\Thermo-Calc\2018a\Examples\Console-mode\Th
SYS: set-echo
SYS: @@
SYS: @@ Plotting thermodynamic functions
SYS:
SYS: @@ This example shows how to plot thermodynamic
SYS: @@ functions in unary, binary and ternary systems.
SYS: @@ It also involves working with partial derivatives
SYS: @@ and partial quantities.
SYS:
SYS: set-log ex02,,
SYS:
SYS: go da
... the command in full is
GOTO_MODULE
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v9.0
```



Drag and drop files into the Console window to open or run a macro, for example. File types that can be opened this way are macro files (*.TCM and *.DCM), database files (*.TDB), and workspace files (*.POLY3, *.GES5, *.PAR, and *.DIC). Note that *.DCM and *.DIC file extensions are applicable to the Diffusion Module (DICTRA). Note that GES6 workspace files cannot yet be dragged and dropped.

Log Files

Log files with the file extension *.TCM are plain text files used to save a sequence of commands. Log files can be edited in a text editor.

- To start saving your input into such a file, use SET_LOG_FILE in the SYS module, followed by the name of the file that you want to save your command sequence to.

- If you want to save the output in the log file as well, use SET_ECHO before the SET_LOG_FILE command. Doing this is useful if you want use the log file later as a macro file.

Macro Files

Macro files (with the file extension of either *.TCM or *.LOG) are plain text files used to save a sequence of commands that can be loaded and executed. Macro files can be edited in a text editor. When creating a command sequence, you add comments to the file by starting a line with @@.

Macro files include comments, which you can either run in Thermo-Calc or open and read in a text editor.



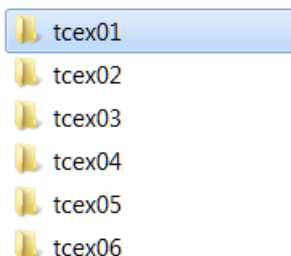
If you only open and read the macro file in a text editor, you do not see the output that Thermo-Calc gives in response to the commands stored in the macro file. It is recommended you run the macro to view all the details.

OPENING A CONSOLE MODE EXAMPLE MACRO FILE

To open an example macro file for Thermo-Calc:

1. Open Thermo-Calc.
2. Confirm you are in Console Mode. If not, click the **Switch to Console Mode** button.
3. From the main menu, select **File →** or **Help → Examples Files**. The Console Mode folder opens.
4. Open the **Thermo-Calc** folder to see the available examples contained in separate folders.

Name





For the Diffusion Module (DICTRA) examples (*.DCM macro files), open the **Diffusion Module - DICTRA** folder.

5. In the folder, double-click the *.TCM file or click **Open**.
6. Follow the prompts in the Console window i.e. keep pressing <Enter> to run the macro and produce a plot in the **Console Results** window.

MACRO FILE COMMANDS

| Action | Command | Description and Comments |
|---------------------------------------|-------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| To load a macro file | In the SYS module, "MACRO_FILE_OPEN" on page 114 followed by the name of the macro file. | Thermo-Calc starts the command sequence that the file contains. |
| Regain control of the console | "SET_INTERACTIVE" on page 119 | End a macro file with this command to have control of the Console returned to you. |
| Add comments to a macro file | Start a line with @@, or enclose it between an @ (-line and a @)-line. | When lines are enclosed the software ignores them when running the macro. |
| Open a macro file | MACRO_FILE_OPEN | When creating the log file, you can make a macro file load up to five other macro files. |
| Nest macro files inside of each other | MACRO_FILE_OPEN SET_INTERACTIVE | If a nested macro file ends with SET_INTERACTIVE, then Thermo-Calc resumes with the higher-level macro file at the command immediately following the MACRO_FILE_OPEN command that loaded and executed macro file that has just been terminated. If a nested macro file doesn't end with SET_INTERACTIVE (but with an end-of-file character), then the console shuts down and the macro is stopped. |

MACRO FILE CONTROL CHARACTERS

The @? character allows you to make a macro interactive by allowing input. At the @? character, which is placed where a parameter value or argument is normally put, Thermo-Calc prompts to input the value of a parameter or argument. You can enter a string

immediately following the @? character. This string is presented to the user when prompted to enter the parameter value or argument. The entered value is used by Thermo-Calc as input to the command in question. For example, you can request the user to specify the temperature range of a stepping calculation by entering the following in a macro file:

```
SET_AXIS_VARIABLE 1 T @?Low-temperature-limit: @?High-temperature-limit:
```

You can also use up to nine variables in your macro file and prompt the user to enter values that can be assigned to these variables. Use the @#n character when you want to prompt the user to provide a value to the variable, where the n is a digit between 1 and 9. You can then use this value by with the ##n character. For example, you can request the user to provide the first element of a system by entering the following in the macro file:

```
@#3First-element?
```

You can then use this variable with the entering the character ##3 later in the macro file. For example, you can write:

```
SET_AXIS_VARIABLE 1 x(##3) 0 1,,,
```

Finally, there is the @& pause character. Thermo-Calc pauses and waits for input from the user when this pause character is read from a macro file. Inserting pause characters is useful if you want to allow the user to monitor what is happening when Thermo-Calc is running the macro.

RESPONSE-DRIVEN MODULES AND MACROS

Macro files that are created while you use a *response-driven module* begin with the module-entering command (for example, `Goto_Module Scheil`) followed by a number of lines with responses to the module's questions and requests. The file terminates with the commands ["POST" on page 175](#) or ["SET_INTERACTIVE" on page 119](#) (this command gives you back control of the Console). An empty line cannot be edited with any input rather than the default answer (to a specific question). Comment lines, commands to open other macro files, pause characters or input-controlling characters cannot be inserted between these empty lines (otherwise the response-driven module cannot be executed properly).

Workspace Files



For DICTRA Console Mode see *File Formats* in the *Diffusion Module (DICTRA) User Guide*

Workspaces files allow you to save all the data in your current workspace. A workspace contains all the data, specified settings and the result of any calculations performed. The

saved data includes original and modified thermodynamic data, the last set of conditions and options, and the results of any simulations. You use the command `SAVE_WORKSPACES` to create this file type, which is available in the POLY, GIBBS and PARROT modules.

When in Thermo-Calc Console Mode these are the workspace file extensions:

- POLY module (*.POLY3)
- GIBBS (GES) module (*.GES5) (This cannot currently be done with GES6)
- PARROT module (*.PAR and *.POP)



For DICTRA in Console Mode, the PARROT module file extension is *.DOP.

The workspace has all the settings specified and the result of any stepping or mapping operations performed after using `SAVE_WORKSPACES`. Consequently, the command opens a workspace in which all data is saved which is generated after the `SAVE_WORKSPACE` command is executed. The saved data includes original and modified thermodynamic data, the last set of conditions and options, and calculation results.

To load the data and calculation results of a workspace file, use the `READ_WORKSPACES` command available in the POLY module. The file can be used for calculation in POLY, visualization in POST, or data manipulation in GES. You are also given the option in the POURBAIX and SCHEIL modules to open a previously saved workspace file. This allows you to make new POURBAIX or SCHEIL calculations on the same chemical system as before but with different temperature, pressure, and composition conditions, or to plot new property diagrams based on the previous calculations.



A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.



Drag and drop files into the Console window to open or run a macro, for example. File types that can be opened this way are macro files (*.TCM and *.DCM), database files (*.TDB), and workspace files (*.POLY3, *.GES5, *.PAR, and *.DIC). Note that *.DCM and *.DIC file extensions are applicable to the Diffusion Module (DICTRA). Note that GES6 workspace files cannot yet be dragged and dropped.

Links to Workspace Commands in Various Modules

POLY MODULE

-
- ["READ WORKSPACES" on page 176](#)
 - ["SAVE WORKSPACES" on page 176](#)

GIBBS (GES) MODULE

- ["READ GES WORKSPACE" on page 241](#)
- ["READ WORKSPACES" on page 241](#)
- ["SAVE GES WORKSPACE" on page 243](#)
- ["SAVE WORKSPACES" on page 243](#)

PARROT MODULE

- ["READ PARROT WORKSPACES" on page 277](#)
- ["SAVE PARROT WORKSPACES" on page 278](#)

ED-EXP MODULE (SUBMODULE TO PARROT)

- ["READ WORKSPACES " on page 304](#)
- ["SAVE WORKSPACES " on page 305](#)

REACTOR MODULE

- ["READ WORKSPACE" on page 346](#)
- ["SAVE WORKSPACES" on page 346](#)

IMPORTANT INFORMATION ABOUT MAP AND STEP COMMANDS AND THE SAVE_WORKSPACES COMMAND



A STEP or MAP command automatically saves the workspace with the most recently specified name. Do not use the SAVE_WORKSPACES command after a MAP or STEP command.

The results from the STEP or MAP commands are destroyed by the SAVE_WORKSPACE command. You can append several results obtained by sequential STEP or MAP calculations without destroying the previous results, whilst SAVE_WORKSPACE erases them all. Keeping this in mind is important and useful particularly for calculating various isothermal (or isoplethal) sections and plotting them on the same diagram in a single Thermo-Calc run.

To suspend some of the STEP or MAP results, use the AMEND_STORED_EQUILIBRIA command.

Editing the Default Console Directory

You can add a startup parameter to a shortcut when launching Thermo-Calc on any of the platforms. When you launch the revised shortcut, the file path is set to a user-defined default directory. An example of why you might want to have a custom directory path is if you use batch projects or if you have macro files for batch jobs. The custom directory file path can also be viewed from within Console Mode.

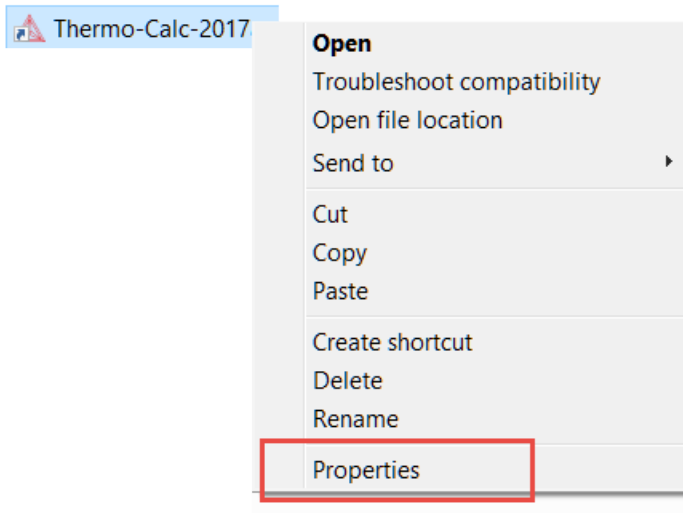


The shortcut is only valid throughout the existing session; it is not saved as a default. Each time you want to use this file path you must launch Thermo-Calc from the customized shortcut.

The following uses Windows for the example.

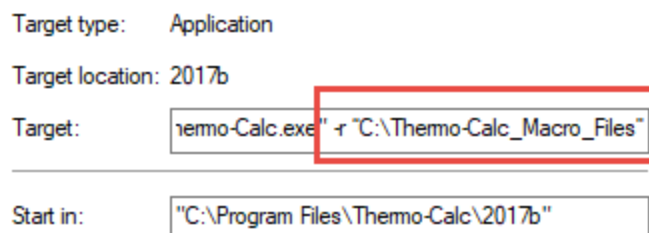
SETTING UP THE DEFAULT CONSOLE DIRECTORY

1. Right-click a shortcut to Thermo-Calc and click **Properties**.



2. In the **Thermo-Calc 2020a Properties** dialog, **Target** field, add the following to the end of the string: `-r` plus the *“path to the default directory”*. Include a space between the `-r` and path, and use quotation marks around the full file path. A simple example:

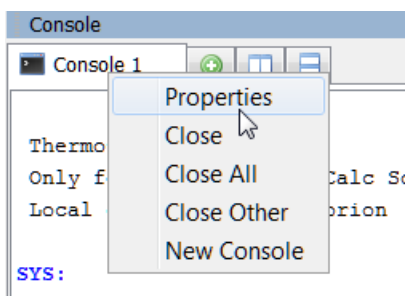
-r “C:\Thermo-Calc_Macro_Files”



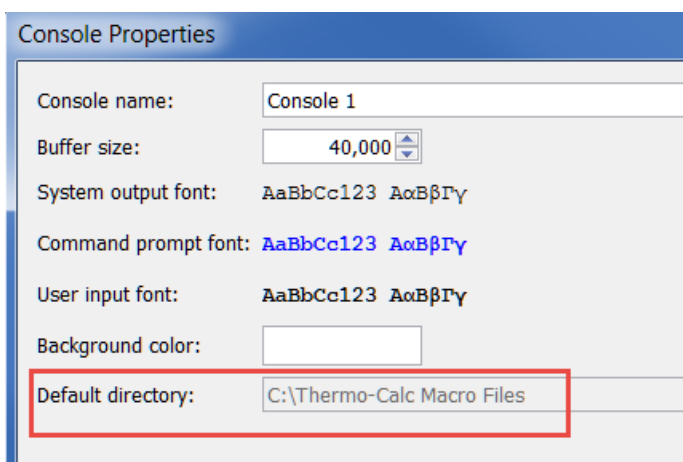
3. Click **Apply** and **OK**.
4. Launch Thermo-Calc from the shortcut where you added the parameter. You can confirm that it is set correctly from within Thermo-Calc.

VIEWING THE FILE PATH IN THERMO-CALC

1. Launch Thermo-Calc from the short cut where you added the parameter.
2. In Console Mode, right click the **Console** window and choose **Properties**.



3. In the **Console Properties** window the **Default directory** section displays the custom file path.



Experimental Data Files (*.POP, *.DOP)



There is also another type of experimental data file (*.EXP) generated when working with DATAPLOT. See ["About the DATAPLOT Graphical Language" on page 3](#).

In order to conduct an assessment for a system, the experimental data is described with a syntax, which is similar to the way that one calculates an equilibrium in the POLY module or you edit an experimental point in the ED_EXP module. Similar to a Thermo-Calc macro file (*.TCM), an experimental data file (i.e. the *.POP or *.DOP file) is a basic text file and can be opened and edited by any text editor. For this reason, a *.POP or *.DOP file is not hardware dependent.

A POP or DOP file consists of various commands from the POLY and ED_EXP modules, as well some special commands which can only be used in such experimental data files. Various experimental information can be inputted in an *.POP or *.DOP file as different tables; the same type of experimental data are usually documented in the same table (see below).

A *.POP or *.DOP file is used in the PARROT module to provide experimental information for the optimization process, and is checked by a *syntax checker* when the PARROT command ["COMPILE_EXPERIMENTS" on page 261](#) is proceeded.

The special commenting identifier, i.e. a dollar sign \$ which starts a line, is used to document comment lines at any position in a *.POP or *.DOP file. You may remember that this feature is universally the same as in almost all kinds of text files in Thermo-Calc software, e.g. in *.TDB, *.DAT, *.TCM, *.POP/*.DOP and *.EXP files. Such a sign and all information afterwards in the same comment line is skipped and ignored by the syntax checker.

Many POLY and ED_EXP commands can be directly used in a POP or DOP file. But there are some differences with the set of POLY or ED_EXP commands, and some specially designed commands as described in this topic can only be used in the *.POP or *.DOP files.

FREQUENTLY USED POLY COMMANDS

Most of the commands in the experimental data file are the same as in the POLY module. The most frequently used are listed below:



The last command in an *.POP or *.DOP file must always be the SAVE command.

- ["CREATE_NEW_EQUILIBRIUM" on page 159](#)
- ["CHANGE_STATUS" on page 152](#)
- ["SET_CONDITION" on page 181](#)
- ["SET_REFERENCE_STATE" on page 185](#)
- ["ENTER_SYMBOL" on page 167](#)
- ["SAVE_WORKSPACES" on page 176](#)

LESS OFTEN USED POLY COMMANDS

Other legal commands from the POLY module that are used less often are:



The DEFINE-COMPONENTS command must be always used as the first command in an *.POP or *.DOP file, as it automatically reinitiates the whole workspace.

- ["DEFINE_COMPONENTS" on page 160](#)
- ["EVALUATE_FUNCTIONS" on page 170](#)
- ["SET_ALL_START_VALUES" on page 178](#)
- ["SET_NUMERICAL_LIMITS" on page 184](#)
- ["SET_START_VALUE" on page 187](#)
- ["ADVANCED_OPTIONS" on page 135](#)

FREQUENTLY USED EDIT EXPERIMENTS (ED_EXP) COMMANDS

Most of the special commands for the ED_EXP module are also often used in an *.POP or *.DOP file. For example:

- ["EXPERIMENT" on page 296](#)
- ["EXPORT" on page 298](#)
- ["IMPORT" on page 299](#)
- ["LABEL_DATA" on page 300](#)
- ["SET_ALTERNATE_CONDITION" on page 307](#)
- ["SET_WEIGHT" on page 316](#)

DO NOT USE THESE EDIT EXPERIMENT (ED_EXP) COMMANDS



The following special ED_EXP commands are illegal and should not be used in any *.POP or *.DOP file:

- COMPUTE-ALL-EQUILIBRIA
- MAKE-POP-FILE
- READ (READ-BLOCK OR READ-WORKSPACE)

-
- TRANSFER-START-VALUES

Calculations

▶ ["Graphical Mode vs Console Mode: Calculation Types" on page 9](#)

In this section:

| | |
|--------------------------------------------------|----|
| About the Gibbs Energy System (GES) Module | 36 |
| Equilibrium Calculations | 38 |
| Property Diagrams | 45 |
| Phase Diagrams | 50 |
| T0 Temperature Simulations | 59 |
| Paraequilibrium | 62 |
| Potential Diagrams | 66 |
| Scheil Simulations | 71 |
| Aqueous Solutions and Pourbaix Diagrams | 81 |
| Tabulation Reactions | 94 |

About the Gibbs Energy System (GES) Module

The Gibbs Energy System (GES) module is an important Thermo-Calc Console Mode module and consists of a comprehensive subroutine package for various thermochemical calculations. The module is interactively connected with all basic and advanced modules in Thermo-Calc and the add-on Diffusion Module (DICTRA). Most users will not directly use the GES module and commands unless you perform assessments.

The GES module is in essence the Thermo-Calc calculation engine, sometimes referred to as the *calculation core*. When working in Graphical Mode you are using the GES calculation engine behind the scenes, whereas in Console Mode, and if you are performing assessments, you are directly interacting with the module. This is also applicable if you are working with any of the software development kits (SDKs).

The objective of the GES module is to provide a unified set of subroutines to be used in any application program that needs thermochemical data. All kinds of thermodynamic models for various types of substances are implemented. However, most model-dependent features are hidden inside the module, and the application programmer can use a standardized set of subroutines, i.e. using the Thermo-Calc SDKs such as TC-Python, TQ-Interface, TC-API and TC-Toolbox for MATLAB® to calculate the integral Gibbs energy or any partial derivative thereof for each phase at any composition, temperature and pressure.

There are subroutines to analytically calculate the first and second partial derivatives of integral Gibbs energy with respect to any variable. You can enter and modify phase descriptions, model connections, basic thermodynamic parameters, and so on.

POLY and all other basic and special modules, as well as the add-on Diffusion Module (DICTRA), interactively call the subroutines within the GES module to calculate any thermodynamic quantities.

Calculation Engine: GES5 vs GES6



GES6 is a re-write and new implementation of the Gibbs Energy System module of Thermo-Calc and it is the default engine. The previous version, GES5, is still available and will continue to work in the background of the program where necessary. The main purpose of GES6 is to support faster development of new features. However, not all GES5 functionality is implemented in GES6. In such cases (except for optimization, PARROT and the POURBAIX module), GES6 falls back silently and uses functionality from GES5 in the background.



To globally set the default from GES6 back to GES5, go to the **Tools → Options** → **"General" on page 37** tab and click **Version 5** for the *Preferred Gibbs Energy System* setting. This is useful if you are using the PARROT module (optimization), POURBAIX module (aqueous solutions), or if you have a custom database that is not compatible with GES6. The **"SET_GES_VERSION" on page 118** Console Mode command can also be used to change GES versions for a single Thermo-Calc session.



Contact Thermo-Calc Software AB at info@thermocalc.com for more information about the changes or if you encounter any issues you think are related to the new version of the calculation engine.

Equilibrium Calculations

In this section:

| | |
|-------------------------------------------------------------------|----|
| The Equilibrium Calculation Module (POLY3) | 39 |
| Setting Conditions for Equilibrium Calculations | 40 |
| Calculating an Equilibrium | 42 |
| Calculating an Equilibrium with a Fixed Phase | 43 |
| Calculating an Equilibrium with Suspended or Dormant Phases | 43 |

The Equilibrium Calculation Module (POLY3)

An equilibrium describes what the composition of the end state of a system is, given a full specification of state variables such as temperature, pressure, initial composition, system size, etc. An equilibrium calculation is normally done in POLY-3 according to the *Global Minimization Technique*, which ensures that the most stable minimum under the specified conditions is computed.

For an equilibrium calculation to be performed, the state variables must all be set as conditions for the calculations. Such conditions include, for example, temperature, pressure, and system composition. When you calculate an equilibrium in the POLY module, you have to set these conditions manually.

Knowledge of the thermodynamic equilibrium is an important factor for understanding properties of materials and processes. With a database of thermodynamic model parameters, it is possible to predict such properties and also to obtain driving forces for diffusion-controlled phase transformations and other dynamic processes.

With the equilibrium calculation module, POLY3, it is possible to calculate many different kinds of equilibria and diagrams, in particular multicomponent phase diagrams.

Different types of databases can be used with the POLY module, and it can be used for alloys or ceramic systems, as well as gaseous equilibria, aqueous solution involved heterogeneous interaction systems. Up to 40 elements and 1000 species can be defined into a single system for equilibrium calculations.

All normal thermodynamic state variables can be used to set as conditions in calculating equilibria, and as axes in plotting diagrams. You can set the composition or any property of an individual phase as a condition. Any state variable can be varied along an axis in order to generate a diagram. During calculations of a diagram, complete descriptions of all calculated equilibria are stored, and in the diagram any state variable can be used as an axis.

The *Global Minimization Technique* is used to ensure that the present minimum in an equilibrium calculation is the most stable minima for the specified conditions. This is based on the traditional GEM (Gibbs Energy Minimization) technique.

A direct global minimization can be performed on conditions: N, n(comp), B, b(comp), w(comp), x(comp), T, and P, but not when combined conditions as e.g. $w(a)-3*w(b)=1$ are used or when an activity or potential condition is used. For all other types of conditions where regular minimization converges, Indirect Global Minimization, i.e. global test and corrections, if necessary, are performed until the lowest minimum is found.

- Direct Global Minimization: From the mesh of Gibbs energy, find the set of grid points that gives the lowest energy solution under the specified conditions. This set of

grid points provides starting combination of phases and their constitutions for regular minimization to find the exact equilibrium solution. This solution is then subject to a global test as described below.

- Indirect Global Minimization: Under certain conditions, a direct approach is impossible. In this case, regular minimization is performed first and then a check is performed in order to see if the found local minimum is a global one by checking if all grid points are above the equilibrium Gibbs energy plane. If not, then recalculate by including these grid points until no grid point is above the equilibrium Gibbs energy plane from the previous step.

The full-scale and full-scope usage of the *Global Minimization Technique* has been extended from for only single-point calculations for all types of calculations (of single-points, property diagram stepping and phase diagram mapping) in Thermo-Calc.

The use of *Global Minimization Technique* may increase the computation time. The main cost in time comes from the calculation of Gibbs energy at each grid point generated by properly meshing the composition space for each entered phase. An additional (but much smaller) cost in time comes from finding the set of grid points in the above mesh that give the lowest energy solution. This solution is where POLY starts its ordinary minimization. When POLY has found an equilibrium, the equilibrium Gibbs energy surface is compared to the mesh to assure that no grid point is below the surface, i.e. a global minimization has been reached.

Global minimization is performed by default in single-point or stepping or mapping equilibrium calculations.

Together with the PARROT module, the POLY module is also used for critical assessment of experimental data in order to develop thermodynamic databases. The POLY module uses the Gibbs Energy System (GES) for modeling and data manipulations of the thermodynamic properties of each phase.

Setting Conditions for Equilibrium Calculations

Setting a condition normally involves giving a single state variable a specific value. For example, you can set the temperature to 1273.5 Kelvin ($T=1273.5$). Alternatively, setting a condition can involve giving a linear expression with more than one state variable a specific value. For example, you can set the mole fraction of the S component to be the same in the liquid and the pyrrhotite phases ($X(\text{LIQ}, S) - X(\text{PYRR}, S) = 0$).

```

POLY_3:1-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium =      1, label A0  , database: TCFE7

Conditions:
T=1000, P=1E5, X(C)=5E-2, N=1
DEGREES OF FREEDOM 0

Temperature 1000.00 K ( 726.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.36552E+01
Total Gibbs energy -4.07975E+04, Enthalpy 2.41176E+04, Volume 7.21740E-06

Component      Moles      W-Fraction Activity Potential Ref.stat
C               5.0000E-02  1.1193E-02 2.1816E-01 -1.2659E+04 SER
FE             9.5000E-01  9.8881E-01 6.1895E-03 -4.2279E+04 SER

BCC_A2                Status ENTERED   Driving force 0.0000E+00
Moles 9.5069E-01, Mass 5.3063E+01, Volume fraction 9.6312E-01 Mass fractions:
FE 9.99844E-01 C 1.55514E-04

GRAPHITE                Status ENTERED   Driving force 0.0000E+00
Moles 4.9313E-02, Mass 5.9230E-01, Volume fraction 3.6881E-02 Mass fractions:
C 1.00000E+00 FE 0.00000E+00

```

The number of state variables that need to set is determined by the *Gibbs Phase Rule*. Typically, the state variables to give values to are:

- temperature (in K)
- pressure (in Pascal)
- system size in number of moles (in mole) or mass (in grams)
- the fraction of each component (in number of moles or mass)

If you fix the phase of the equilibrium and all but one of the state variables, you can discover the value of the other state variable at equilibrium.

It is possible to specify a set of conditions that does not have any equilibrium and the program detects this by failing to reach equilibrium during the calculation.

STATE VARIABLES

The following table lists some of the available state variables you can use to set conditions:

| State Variable | SET_CONDITION Parameter |
|------------------------------------|-------------------------|
| temperature in the system (in K) | T |
| pressure in the system (in Pascal) | P |

| State Variable | SET_CONDITION Parameter |
|-----------------------------------------------------------------------------------------|-------------------------|
| system size (mole number in moles) | N |
| system size (mass in grams) | B |
| number of moles of a component in the system | N(<component>) |
| mole fraction of a component in the system | X(<component>) |
| mass fraction of a component in the system | W(<component>) |
| activity of a component in the system | ACR(<component>) |
| chemical potential of a component in the system | MUR(<component>) |
| mole fraction of a component in a phase | X(<phase>,<component>) |
| mass fraction of a component in a phase | W(<phase>,<component>) |
| activity of a species referred to a phase at ambient temperature and pressure | ACR(<species>,<phase>) |
| chemical potential of a species referred to a phase at ambient temperature and pressure | MUR(<species>,<phase>) |
| enthalpy in the system (in J) | H |
| enthalpy of a phase (in J/mol) | HM(<phase>) |

Calculating an Equilibrium

This topic explains how to calculate an equilibrium in POLY. To calculate an equilibrium means to calculate the equilibrium composition of your system, given a full specification of conditions that reduce the degrees of freedom of the calculation to zero.



If you are running a network client installation of Thermo-Calc and cannot enter the POLY module, this may be because all the license instances on that the license server makes available have been checked out.

▶ ["POLY Module Commands" on page 131](#)

1. Define your system.



["Defining a System in Console Mode" on page 8](#)

2. Go to the POLY module. At the SYS prompt, type `GOTO_MODULE` and enter `POLY`.

-
3. Use `SET_CONDITION` followed by conditions and value assignments to set the conditions of your calculation. For example, to set temperature, pressure, initial composition and system size for a Fe-Cr-C system, you might enter the following:

```
SET_CONDITION T=1200 P=1E5 W(CR)=0.18 W(C)=0.0013 N=1
```

This sets the temperature (T) to 1200 K, the pressure to 1 bar (100,000 Pascal), the mass fraction of Cr to 18 mole percent, the mass fraction of C to 0.13 weight percent, and the total amount of material to 1 mole. The fraction of Fe in the system is calculated from the fractions of Cr and C. You have to set the fraction of all the components in your system except one.

4. Use `COMPUTE_EQUILIBRIUM` to run the calculation.
5. Use `LIST_EQUILIBRIUM` to see the results of the calculation.

Calculating an Equilibrium with a Fixed Phase

There are many ways to calculate equilibriums in Thermo-Calc. The following is one example.

You can calculate an equilibrium that has a certain amount of a certain stable phase. Use ["CHANGE_STATUS" on page 220](#) and choose `Phase` to specify the phase and the amount of that phase (in normalized mole number) that you want to set as fixed. For example, if you want to find out at what temperature a system starts to melt, enter the following:

```
CHANGE_STATUS PHASE LIQUID=FIX 0
```

You must leave the state variable whose equilibrium value you are interested in unspecified. However, if you have already specified that state variable, you can make it unspecified again by using ["SET_CONDITION" on page 181](#) and set that state variable to `NONE`. For example, if you have given temperature a value, you can type:

```
SET_CONDITION T=NONE
```

The calculated equilibrium includes the value of the unspecified variable at which the equilibrium enters the phase that is fixed.



For an example where an equilibrium is calculated with a fixed phase, see Console Mode example `tcex07`.

Calculating an Equilibrium with Suspended or Dormant Phases

You can calculate an equilibrium under the assumption that one or several phases are `SUSPENDED` or `DORMANT` using `CHANGE_STATUS` and choose `Phase`. For example, to specify that all phases except one should be suspended, you can first suspend all phases and then enter a

single phase in the following way:

```
CHANGE_STATUS PHASE *=SUSPENDED  
CHANGE_STATUS PHASE FE_LIQUID=ENTERED
```



For an example where this is done, as well as where the status of phases is set to be dormant, see the ["Single Equilibrium Calculation Examples" on page 432](#).

Property Diagrams

In this section:

| | |
|----------------------------------------------------------|----|
| About Property Diagrams | 46 |
| Calculating and Plotting a Property Diagram | 46 |
| Calculating a Property Diagram One Phase at a Time | 48 |
| Calculating Several Properties in the Same Diagram | 49 |

About Property Diagrams

When you calculate and plot a property diagram, there is only one independent state variable. Many different properties can be plotted as a function of this independent variable. For example, if the independent state variable is temperature, then the mole fractions of all phases can be plotted as a function of temperature. Or the composition of a specific phase may be plotted relative to temperature, or the activity of a component in the system as a whole or in a specific phase may be plotted relative to it.

A property diagram is plotted based on a series of equilibria that is computed while the value of one state variable is varied between a minimum and a maximum value. This variable is referred to as the stepping axis variable. In Thermo-Calc, first calculate one initial equilibrium, and then new equilibria are calculated at incremental steps in both directions on the stepping axis from the initial equilibrium. This continues until the stepping operation has covered the length of the axis between a minimum and a maximum value that is specified.



For an example of the calculation of a property diagram, see [tcex08](#).

Calculating and Plotting a Property Diagram

This topic explains how to calculate a property diagram in POLY. To calculate a property diagram means to calculate a series of equilibria while the value of the stepping axis variable varies between a minimum and a maximum value. With the exception of the stepping axis variable, all the state variables that you set when you calculate the initial equilibrium retain the values when the new equilibria are calculated.



["POLY Module Commands" on page 131](#)

1. Calculate an initial equilibrium in the POLY module.
2. Use SET_AXIS_VARIABLE to set the axis variable, the minimum and the maximum stepping variable values and the step length. The first parameter of SET_AXIS_VARIABLE is the axis number. Since a property diagram only has one axis variable, this is set to 1. For example, if you want to set the axis variable to temperature, and calculate an equilibrium at every 50 K between a minimum temperature of 100 K and a maximum temperature of 2000 K, enter

```
SET_AXIS_VARIABLE 1 T 100 2000 50
```




An axis variable must be a state variable that is set when you calculated the initial equilibrium. For example, if you set the fraction of a component in number of moles, then you cannot set the mass fraction of this component as an axis variable. Also, the minimum stepping variable value must be smaller than, and the maximum value larger than, the value that you set the state variable to when calculating the initial equilibrium.

3. Use STEP_WITH_OPTIONS and choose `Normal` to perform the stepping operation.

Thermo-Calc lists the phase regions along the stepping axis, the phases contained in each region, and the number of equilibria calculated in that region. Each region is defined by the phases it contains.



The number of equilibria calculated is not just the number of steps that are performed according to the step length and the minimum and maximum values on the axis variable. This is because Thermo-Calc calculates extra equilibria when a new phase is discovered in order to determine the phase region boundary more precisely.

```

POLY_3:s-a-v 1 T 1000 2000 100
POLY_3:step
Option? /NORMAL/:
  No initial equilibrium, using default
  Step will start from axis value    1000.00
...OK

Phase Region from    1000.00    for:
  BCC_A2
  GRAPHITE
Global check of adding phase at  1.01118E+03
Calculated    4 equilibria

Phase Region from    1011.18    for:
  BCC_A2
  FCC_A1
  GRAPHITE
Calculated    2 equilibria

Phase Region from    1011.18    for:
  FCC_A1
  GRAPHITE
Global test at  1.09000E+03 .... OK
Global check of removing phase at  1.15727E+03
Calculated    17 equilibria

```

4. To plot the diagram, use POST to open the POST module and then use PLOT_DIAGRAM. By default, the X-axis represents the stepping axis variable and Y-axis represents the sum of the mole fractions of all phases (NP(*)).

Calculating a Property Diagram One Phase at a Time

There are many ways to calculate property diagrams in Thermo-Calc. One example is where you can calculate a property diagram with a separate stepping operation being performed for each phase at a time in its default most stable composition (the major constitution). This is useful if you want to create a property diagram for a heterogeneous system with both ordered phases and their disordered pairs.

To calculate a property diagram one phase at a time, use ["STEP WITH OPTIONS" on page 188](#) and when prompted choose `One_phase_at_time` to perform the stepping operation.

Calculating Several Properties in the Same Diagram

There are many ways to calculate property diagrams in Thermo-Calc. The following is another example. If you perform several stepping calculations after each other, the results of these calculations are all saved in your workspace file. This allows you to the following:

- Calculate (and then plot) missing parts of a specific property inside the first property diagram. These parts are calculated inside the range of the stepping variable with a different control condition.
- Calculate (and then plot) two or more sets of a specific property on the same property diagram for the same system. These can be calculated under different control conditions with stepping operations being performed across the same stepping axis variable range.
- Calculate phase boundary lines and then plot them in a corresponding phase diagram for the same system. This can be especially useful for some defined secondary phase-transformations. For example, if you want to find the phase boundary between BCC_A1 and BCC_B2, or the equal-Gm for two specific phases, or the equal-fraction or equal-activity for two specific phases of a certain species, then this can be useful.

Unless you have opened a new workspace file previously using `SAVE_WORKSPACES`, the results of the stepping calculations are saved in a `RESULT.POLY3` file. To save the results of several stepping calculations in a file different from the workspace file that your results are currently saved to, then use `SAVE_WORKSPACES` before you perform the first stepping calculation.



`SAVE_WORKSPACES` overwrites and deletes the results of all previous stepping calculations.



A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

Phase Diagrams

In this section:

| | |
|-----------------------------------------------------------|----|
| About Phase Diagrams | 51 |
| About Binary Phase Diagrams | 53 |
| About Ternary Phase Diagrams | 54 |
| About Quasi-Binary and Quasi-Ternary Phase Diagrams | 56 |

About Phase Diagrams

Phase diagrams have two or more independent axis variables. Any state variable that has already been set can be used as the mapping variable for a mapping calculation and then as the axis variable for a phase diagram. From a mapping calculation, many types of phase diagrams can be plotted, with one of the mapped variables as one axis variable, and with other mapped variables or any varied property (state or derived variables) or entered symbol (variables, functions or table values) as the other axis variables.

All phase diagrams consist of zero phase fraction lines. There are two distinct types of phase diagrams: those with the tie-lines in the plane of the diagram and those where the tie-lines are not in the plane. The former includes binary phase diagrams and ternary isotherms. The latter includes more general isopleth diagrams with one or more fixed extensive variables (normally, this is a composition).

- The BIN and TERN modules calculate binary and ternary phase diagrams.
- The POTENTIAL and POURABIX modules calculate the more general isopleth diagrams and other related diagrams.

The following topics describe how to calculate the types of phase diagrams in the POLY_3 module. In POLY, you can calculate phase diagram for systems with up to 40 components and with thousands of phases. You can combine activity conditions and fixed phase status and fraction conditions in any way. Thermo-Calc can calculate any arbitrary 2D section through composition space.



There is no guarantee that the conditions set will result in a calculation that reaches an equilibrium.

- ▶ ["Binary Phase Diagram Examples" on page 415](#)
- ▶ ["Ternary Phase Diagram Examples" on page 423](#)
- ▶ [" Potential Diagram Example" on page 434](#)
- ▶ ["Pourbaix Module Examples" on page 444](#)

Calculating and Plotting a Phase Diagram

This topic describes how to calculate a phase diagram in the POLY module. The commands are described in ["POLY Module Commands" on page 131](#) and ["POST Module Commands" on page 350](#).

-
1. Calculate an initial equilibrium in the POLY module.
 2. Use SET_AXIS_VARIABLE to set the first axis variable, its minimum and maximum mapping value and the length of each incremental step on this axis. The first parameter of SET_AXIS_VARIABLE is the axis number and is set to 1. For example, suppose you want the mass fraction of C as your first axis variable. You want it to vary between 0 and 0.1, with the length of each incremental step being no more than 0.002. You then enter:

```
SET_AXIS_VARIABLE 1 W(C) 0 .1 0.002
```



An axis variable must be a state variable that is set when you calculated the initial equilibrium. For example, if you set the fraction of a component in number of moles, then you cannot set the mass fraction of this component as an axis variable.

3. Use SET_AXIS_VARIABLE to set the second axis variable and specify its minimum, maximum, and step length values. The axis number is set to 2. For example, suppose you want temperature as your second axis variable and you want it to vary between 900 K and 1900 K, with an incremental step of 25 K. You then enter:

```
SET_AXIS_VARIABLE 2 T 900 1900 25
```

4. If you want more than two axis variables, then use SET_AXIS_VARIABLE until you have set all the axis variables. You can set up to five axis variables. Axis variables 3, 4 and 5 must be set temperature, pressure or to the chemical potentials of components.

You may want to save your workspace with SAVE_WORKSPACES before you perform the mapping calculation. This saves the axis variables you have set. However, it overwrites the results of any previous stepping or mapping calculations done.

5. Use MAP to perform the mapping calculation. The console lists the phase region boundaries and the phases contained on one side of each boundary.

```

Phase region boundary 30 at: 1.363E+03 2.012E-01
    FCC_A1
    ** GRAPHITE
Calculated.                3 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 1.990E+03 2.526E-01
    LIQUID
    ** GRAPHITE
Calculated.                13 equilibria
Terminating at known equilibrium

```

6. To plot the diagram, use POST to open the POST module and then use PLOT_DIAGRAM. By default, the X-axis represents mapping axis variable 1 and the Y-axis represents mapping axis variable 2.

About Binary Phase Diagrams

Binary phase diagrams are by far the most common found in the literature and calculated by computers. However, most real systems have more than two components and thus binary diagrams are more a kind of exercise in order to calculate more realistic phase diagrams.

You can calculate many types of binary phase diagrams with POLY, but the traditional one has one composition axis and the temperature on the other axis. This is calculated by first specifying a single equilibrium by setting conditions such as

```
SET_CONDITION T=1200, P=1E5, W(C)=.02, N=1
```

This means that the temperature should be 1200 K, pressure 1 bar, mass fraction of C is 0.02 (i.e., 2 weight percent) and the system contains one mole of atoms. Note that one does not set a condition on the amount of the second component. This is simply taken to be the rest of the system.

After setting these conditions one can calculate the equilibrium by giving the command:

```
CALCULATE_EQUILIBRIUM
```

When the calculation has converged, one continues by setting the axes for the diagram calculation. In most cases, one is interested in the complete composition range but the temperature range may vary.

```
SET_AXIS_VARIABLE 1 W(C) 0 .1 0.002
SET_AXIS_VARIABLE 2 T 900 1900 25
```

This means that the axis number 1 is taken to be the mass fraction of C which may vary between 0 and 0.1 with a maximum increment of 0.002. The axis number 2 is the temperature varied between a minimum 900 and maximum 1900 K with a maximum increment of 25.

Before starting the mapping, it is a good rule to SAVE the workspaces. If this is done just before the MAP command, and the MAP command fails for some reason, the user can restart from the situation just before mapping and try to find a better start point.

```
SAVE
```

```
MAP
```

The diagram is plotted in the post-processor. The post-processor will automatically set the same axes for plotting as used for mapping.

```
POST
```

```
PLOT
```

BINARY_DIAGRAM

The BINARY_DIAGRAM module (short name, the BIN module) enables you to quickly calculate a simple binary phase diagram. Access to specific databases designed for BIN, such as TCBIN, is required.

To enter the module, at the SYS prompt type `GOTO_MODULE BINARY`. There are no other commands for this module. Follow the prompts to plot a diagram.

| Syntax | BINARY_DIAGRAM |
|---------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | Database: /TCBIN/ First element Second element Phase diagram, Phase fraction (FE), G- OR A-curves (G/A): /Phase_Diagram/ |

About Ternary Phase Diagrams

There are many types of ternary phase diagrams but perhaps the most common is the isothermal section. In this case, the temperature is constant, which means that the tie-lines are in the plane of the calculation. Isothermal sections and monovariant lines on the liquidus surface can be calculated in traditional way. They can also be calculated in the TERN module, but this requires a special database (such as PTERN).

In order to set up calculation of a ternary isothermal section in the system Al-Mg-Si, do the following (after retrieving the data from the database (TDB) module):

```
SET_CONDITION T=823,P=1E5,N=1,X(MG)=.01,X(SI)=.01
```

C_E

Note that there is no condition on the amount of Al as that is the "rest". N=1 specifies that the system is closed. This calculation gives one point inside the system. Now define the axis:

```
S-A-V 1 X(MG) 0 1 0.01
S-A-V 2 X(SI) 0 1 0.01
```

Of course, you might not be interested in the whole section, and in such cases specify different lower and upper limits for the axes. Then give a SAVE command before the MAP command:

```
SAVE almg2si-823
MAP
```

The result can be plotted in the POST module. Ternary isopleths are equally simple to calculate. Use the same conditions as above if you are interested in a section of Al-Si at 1 mole percent of Mg, just define a different set of axis:

```
S-A-V 1 X(SI) 0 1 .01
S-A-V 2 T 500 2000 25
SAVE almg2si-1mg
MAP
```

In the resulting diagrams, the tie-lines are not in the plane of the diagram, thus the lever rule etc. cannot be applied. But you can calculate more elaborate sections. An interesting diagram is the section from pure Al to Mg₂Si, which is almost a quasi-binary section. In order to calculate this, set up the conditions differently:

```
SET-CONDITION T=823, P=1e5, N=1, X(MG)-2*X(SI)=0, W(MG)=.01
C-E
```

Note that there is no condition on the amount of Si as this is given by the relation $X(\text{MG})-2X(\text{SI})=0$. Also note that you can mix conditions in X and in W. Then set the axis, save the workspace and map.

```
S-A-V 1 W(MG) 0 .1 .01
S-A-V 2 T 500 1500 10
SAVE al-mg2si
MAP
```

A special type of ternary phase diagrams is liquidus surfaces. This is still not simple to calculate as a separate start point is needed for each separate line at each temperature.

However, you can easily calculate the monovariant lines where the liquid is stable together with two condensed phases:

```
SET-CONDITION T=800, P=1e5, N=1, X(MG)=0.01, X(SI)=.01
```

```

C-E
C-S P LIQ=FIX 0.3
S-C T=NONE
C-E

```

Now there should be an equilibrium where liquid is just stable. Set the axis to be the compositions.

```

S-A-V 1 X(MG) 0 1 .01
S-A-V 2 X(SI) 0 1 .01
SAVE almgsl-luni
MAP

```

TERNARY_DIAGRAM

The TERNARY_DIAGRAM module (short name, the TERN module) enables you to quickly calculate a simple ternary phase diagram.

To enter the module, at the SYS prompt type GOTO_MODULE TERNARY. There are no other commands for this module. Follow the prompts to plot a diagram.

| Syntax | TERNARY_DIAGRAM |
|---------|-------------------------------------------------------------------|
| Prompts | Database: /FEDEMO/ |
| | First element: |
| | Second element: |
| | Third element: |
| | Phase diagram, Monovariants, or Liquidus Surface: /Phase_Diagram/ |
| | Temperature (C) /1000/ |
| | Global minimization on: /Y/ |

About Quasi-Binary and Quasi-Ternary Phase Diagrams

Quasi-binary diagrams, as well as quasi-ternary diagrams and so forth, have often been misunderstood and misused. A real quasi-binary phase diagram is for a ternary system where one component has a fixed activity or chemical potential, and a real quasi-ternary phase diagram is for a quaternary system where one component has a fixed activity or chemical potential.

A typical example of quasi-ternary system is a quaternary system Fe-Cr-Ni-C calculated at fixed carbon activity. The condition can be set as follows:

```

SET-REF-STATE C GRAPH , , , ,
SET-CONDITION T=1273, P=1e5, N=1, X(CR)=.1, X(NI)=.1, ACR(C)=.002

```

In some cases, the activity may vary in a quasi-binary section if one has a phase fixed instead (and where the phase may vary in composition). The advantage with the quasi-binary section is that the tie-lines will be in the plane of the diagram and thus the lever rule etc is obeyed.

A quasi-binary section in Ca-Fe-O when the liquid oxide is in equilibrium with liquid Fe can be specified as follows:

```
DEFINE-COMPONENTS CAO FE FEO
SET-CONDITION T=1850, P=1e5, N=1, X(CAO)=.1
CHANGE-STATUS PHASE FE-LIQ=FIX 0
```

and the mapping can be done with the following axis

```
S-A-V 1 X(CAO) 0 1 .01
S-A-V 2 T 1500 2000 25
```

However, it is a problem as FE-LIQ is not the stable phase for pure iron below 1811. One will have to calculate separate sections depending on the stable modification of Fe.

Calculating a Quasi-Binary Phase Diagram

There are many ways to calculate phase diagrams in Thermo-Calc. The following is an example where a quasi-binary phase diagram is used for calculations on a ternary system in which one component has an activity or chemical potential that is fixed (although if you have fixed a phase and the phase composition varies, then the activity or chemical potential may also vary). The tie-lines in a quasi-binary diagram are in the diagram's plane of the diagram. This means that the calculation follows the lever rule as well as other rules.

When calculating a quasi-binary phase diagram it is necessary to set a condition on either activity or chemical potential of the third component. To specify a meaningful value it is recommended that you first change the component's reference state using SET_REFERENCE_STATE. For example, to calculate a phase diagram for a quasi-binary Fe-Cr-O system with fixed oxygen activity, you can enter the following:

```
SET_REFERENCE_STATE O GAS , ,
```

You must also use SET_CONDITION to set the activity of the component whose activity or chemical potential you have fixed. Do this by assigning a value to the ACR state variable. For example, if the component is oxygen, you might enter

```
SET_CONDITION ACR(O)=0.2
```

ALTERNATIVE WAY TO SET THE COMPONENT ACTIVITY

As an alternative to set the activity of the component, you can Use CHANGE_STATUS to set a

phase to fixed. For example, suppose you want to compute the iron-saturated section in "FeO"-SiO₂. You then enter:

```
CHANGE-STATUS FCC=FIX 0
```

Calculating a Quasi-Ternary Phase Diagram

There are many ways to calculate phase diagrams in Thermo-Calc. The following is an example of a quasi-ternary phase diagram used for calculations on a quaternary system where one component has a fixed activity or fixed chemical potential.

When calculating a quasi-ternary phase diagram it is necessary to set a condition on either activity or chemical potential of the fourth component. To specify a meaningful value it is recommended that you first change the component's reference state using SET_REFERENCE_STATE. For example, to calculate a phase diagram for a quasi-ternary Fe-Cr-Ni-C system with fixed carbon activity, you can enter the following:

```
SET_REFERENCE_STATE C GRAPH , ,
```

You must also use SET_CONDITION to set the activity of the component whose activity or chemical potential you have fixed. Do this by assigning a value to the ACR state variable. For example, if the component is carbon, you might enter

```
SET_CONDITION ACR(C)=0.002
```

T0 Temperature Simulations

In this section:

| | |
|------------------------------------------|----|
| About T0 Temperature Simulations | 60 |
| Making a T0 Temperature Simulation | 60 |

About T₀ Temperature Simulations

The T₀-temperature is the temperature at which two phases have the same Gibbs energy for a certain composition in a multicomponent system. The T₀-temperature is located within the two-phase field between the phases and it is the theoretical limit for a transformation without diffusion. T₀ temperatures are often of interest if you want to understand how diffusionless transformations work. The T₀ temperature in a multicomponent system with a fixed composition is temperature at which the tangent lines of the Gibbs energies of the two target phases are the same.

If the composition of one or two components varies, the common Gibbs energy for the two phases in partial equilibrium of a diffusionless transformation becomes a plane or surface, and the T₀ temperature becomes a line or plane.



See Console Mode examples tcex 23 and tcex41.

Making a T₀ Temperature Simulation

This describes how to perform a T₀ temperature simulation and apply a stepping calculation to its initial result.

Before you perform a T₀ temperature calculation, you must have defined your initial system and be in POLY. The initial overall composition must have appropriate settings for the desired T₀ temperature calculation for the two target phases.



["POLY Module Commands" on page 131](#)

1. Use SET_CONDITION to set the conditions of your calculation in the same way as when you calculate an ordinary equilibrium.
2. Use COMPUTE_EQUILIBRIUM to run the calculation. The calculation does not need to reach an equilibrium in which any of the target phases is stable.
3. When you have calculated your initial equilibrium, use ADVANCED_OPTIONS and choose T-zero.
4. When prompted, specify the names of the two target phases for which the T₀ temperature (where the phases' Gibbs energies are equal) is to be calculated.
5. If the T₀ temperature between the two target phases is calculated, this temperature (in Kelvin) is shown in the Console window.
6. If you want to do a stepping calculation based on this initial T₀ temperature calculation, then use SET_AXIS_VARIABLE to specify which state variable to use as the stepping variable. This is done the same way as when you calculate a normal property diagram.



When a T0 temperature simulation is run, you cannot set temperature as the stepping variable.

7. Use STEP_WITH_OPTIONS and choose T-zero to initiate the stepping calculation. You are prompted to specify the names of the target phases for which the T0 temperature is calculated.

During the STEP T-ZERO calculation procedure, the calculated T0 values are presented next to the stepping variable.

For example, part of the output might look like this:

```
Phase Region from 1.000000E-01 for:
BCC_A2
FCC_A1
1.000000E-01      940.24
9.250000E-02      941.20
2.500000E-03      977.61
7.500000E-09      979.34
```

When the stepping calculation has finished, you can move to the POST module and plot the T0 line against the stepping composition variable or another varying axis value. Or you can impose the calculated T0 line onto a normal phase diagram.

Paraequilibrium

In this section:

| | |
|-------------------------------------|----|
| About Paraequilibrium | 63 |
| Calculating a Paraequilibrium | 63 |

About Paraequilibrium

A paraequilibrium is a partial equilibrium where one interstitial component (such as carbon C and nitrogen N) in a multicomponent alloy can diffuse much faster than the other components (the substitutional elements, including the matrix element and alloying elements). The chemical potential for the interstitial component in two partially equilibrated phases is equal in such a case, but this is not true for the other components. In such a paraequilibrium state, it is possible to have a transformation that is partly without partitions, where a new phase of the mobile component can form with different content but where the slowly diffusing components retain their compositions.

A paraequilibrium calculation is useful when, for example, you want to study phase transformations in systems with large differences in the diffusivities of different elements. Transformations occurring under paraequilibrium states can be much more rapid than if full local equilibrium holds at the phase interface.

► ["Calculating a Paraequilibrium" below](#)

Calculating a Paraequilibrium

This topic describes both how to calculate an initial paraequilibrium with two target phases, and how to base a stepping calculation on this initial calculation.

Before you do any paraequilibrium calculations, you must have defined your initial alloy system and be in POLY. The initial overall composition must have appropriate settings for the desired paraequilibrium calculation for the two target phases.

1. Use ["SET_CONDITION" on page 181](#) to set the conditions of your calculation just like when you calculate an ordinary equilibrium.
2. Use ["CHANGE_STATUS" on page 152](#) to set the status of the chosen interstitial components to SPECIAL. For example, if C is an interstitial component, enter:

```
CHANGE_STATUS COMPONENTS C=SPECIAL
```

This gives you a clear picture on u-fractions of the substitutional and interstitial components, which are different from the overall composition in the system. The SPECIAL status means that the specified components are not included in summations for mole or mass fractions. Therefore, all the composition variables plotted from paraequilibrium calculations are u-fraction related quantities.

3. Use ["COMPUTE_EQUILIBRIUM" on page 156](#) to run the calculation.
4. When you have calculated your initial equilibrium, use ["ADVANCED_OPTIONS" on page 135](#) *Paraequilibrium* to perform the paraequilibrium calculation.

-
5. Specify the names of the target phases of the paraequilibrium state. For example, FCC#1 BCC and FCC#2 M23C6.



Both phases must have similar interstitial/vacancy sublattices that the fast-diffusion interstitial components occupy. Both target phases should have phase constitution definitions that cover all the defined substitutional and interstitial components of the current alloy system.

6. Specify the names of one or more fast-diffusing components. These components must be located on the interstitial/vacancy sublattices in both of the chosen phases.



Interstitial components (for instance C and N combined) may have significantly different behaviours depending on how they are partitioned in different structured phases.

If the paraequilibrium between the two specified phases is successfully calculated, then a message is displayed, for example:

```
NP(FCC) = 0.3586 with U-fractions C = 2.71821E-02 N = 4.1548129E-03
```

```
NP(BCC) = 0.6414 with U-fractions C = 7.10061E-04 N = 2.3781027E-04
```

```
All other compositions are the same in both phases
```

The first two lines show the phase amounts expressed in mole-percent [NP(phase)] and the contents of the interstitial components C and N in each phase. These contents are expressed in u-fractions. The third line states that the compositions of the matrix component and all the remaining compositions (regarding substitutional components) are equal in the two target phases at the paraequilibrium state.

7. If you want to do a stepping calculation based on this initial paraequilibrium, then use ["SET_AXIS_VARIABLE" on page 180](#) to specify which state variable to use as the stepping variable. This is done exactly in the same way as when you calculate a normal property diagram.
8. Use ["STEP_WITH_OPTIONS" on page 188](#) → `Paraequilibrium` to initiate the stepping calculation. You are prompted to specify the names of the target phases of the paraequilibrium states as well as the fast-diffusing components.

The stepping calculation is performed, and the different phase regions are listed with columns for the value of the stepping variable, the amounts of the two target phases, the u-fractions of interstitial(s) in each of the two phases, and the LNACR value(s) of the interstitial component(s).

This command calculates a paraequilibrium between two phases.
 You must calculate an equilibrium with the overall composition first.
 Name of first phase: fcc_a1
 Name of second phase: bcc_a2
 Fast diffusing component: /C/: C
 Fast diffusing component: /NONE/:
 Output during stepping is:
 axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
 and LNACR value(s) of interstitial(s)

```
Phase Region from    900.000    for:
  BCC_A2
  FCC_A1
9.000000E+02    0.176    0.824    4.977501E-02    6.609390E-04    -2.303643E-01
8.900000E+02    0.161    0.839    5.421135E-02    6.889794E-04    -1.689777E-02
8.800000E+02    0.148    0.852    5.872152E-02    7.140931E-04    1.943989E-01
8.700000E+02    0.137    0.863    6.329608E-02    7.362105E-04    4.040959E-01
8.600000E+02    0.127    0.873    6.792661E-02    7.552871E-04    6.126989E-01
8.500000E+02    0.119    0.881    7.260558E-02    7.713010E-04    8.206607E-01
8.400000E+02    0.111    0.889    7.732629E-02    7.842505E-04    1.028392E+00
8.300000E+02    0.105    0.895    8.208278E-02    7.941530E-04    1.236267E+00
8.200000E+02    0.099    0.901    8.686971E-02    8.010431E-04    1.444633E+00
8.100000E+02    0.093    0.907    9.168236E-02    8.049714E-04    1.653814E+00
8.000000E+02    0.089    0.911    9.651648E-02    8.060032E-04    1.864114E+00
```



It is possible to now move to the POST module and plot some of the results of the calculation. For an example of a paraequilibrium calculation and how it can be plotted, see Console Mode example tcex23.

Potential Diagrams

In this section:

| | |
|---------------------------------------------------------------|----|
| About Potential Diagrams | 67 |
| POTENTIAL_DIAGRAM | 67 |
| Calculating a Potential Diagram | 68 |
| Calculating a Potential Diagram with Different Pressure | 69 |

About Potential Diagrams

If you have a metal-oxide/sulphide-gas interaction system, you might want to calculate a so-called potential phase diagram given certain temperature and pressure. A potential diagram uses the activities of two major species in the gaseous mixture phase as mapping variables. The activities (that is, the fugacities at 1 bar) of these two species are typically set as the X- and Y-axis when the diagram is plotted. The phase relations between the gaseous mixture and various metal forms, metal-oxides, metal-sulphides, or other metal-bearing solids, are represented by different fields controlled by these two potential quantities.

This topic describes how to calculate such potential diagrams with the POTENTIAL module, and how to later modify the pressure of such a calculation in POLY. The calculation done by the POTENTIAL module always assumes a pressure of 1 bar.

POTENTIAL_DIAGRAM

The POTENTIAL_DIAGRAM (POT or POTENTIAL) module is a potential phase diagram calculation module.

If you have a metal-oxide/sulphide-gas interaction system, you might want to calculate a so-called potential phase diagram given certain temperature and pressure. A potential diagram uses the activities of two major species in the gaseous mixture phase as mapping variables. The activities (that is, the fugacities at 1 bar) of these two species are typically set as the X- and Y-axis when the diagram is plotted. The phase relations between the gaseous mixture and various metal forms, metal-oxides, metal-sulphides, or other metal-bearing solids, are represented by different fields controlled by these two potential quantities.

To enter the module, at the SYS prompt type `GOTO_MODULE POTENTIAL`.



There are no commands for this module. Follow the prompts and see ["About Potential Diagrams" above](#) for details about how to calculate using potential diagrams.

| Syntax | POTENTIAL_DIAGRAM |
|---------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | Database: /POT/ Press <Enter> and the program lists the available databases. Type one of the database names and press <Enter> to select. The following default elements are then based on the chosen database. Matrix element: /Fe/ First potential species: /S1O2/ Second potential species: /O2/ |

| | |
|--------|---------------------|
| Syntax | POTENTIAL_DIAGRAM |
| | Temperature: /1000/ |

Calculating a Potential Diagram

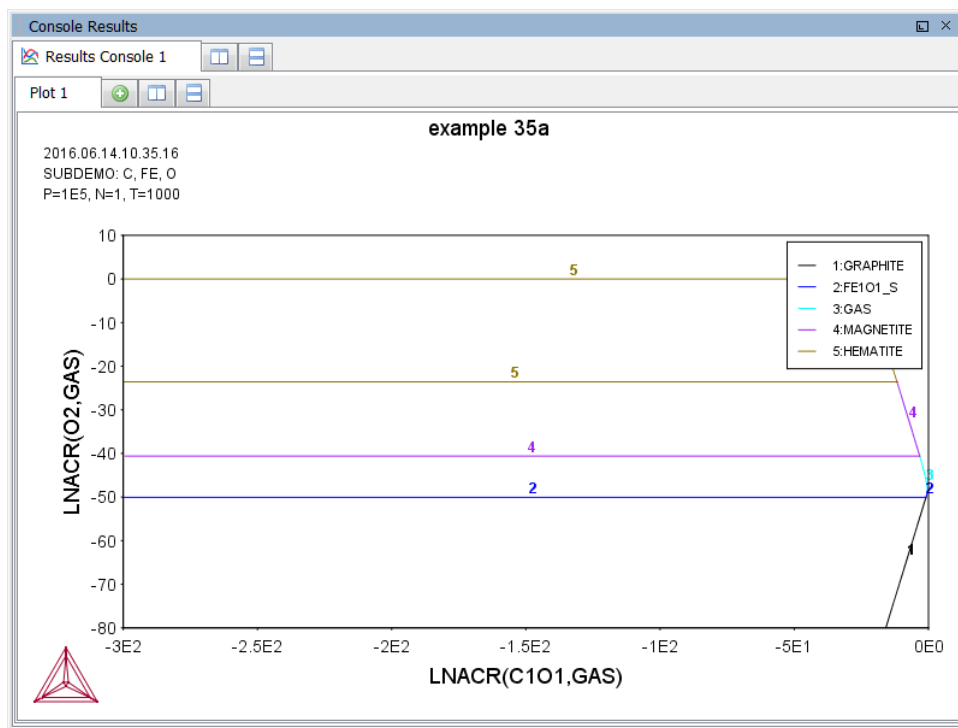
You need access to a substance or solution database that contains a gaseous mixture phase, metals (or alloys), and solids such as metal-oxides, sulphides, sulphates, carbonates, silicates, nitrides or nitrates (stoichiometric or solution phases).

1. Use GOTO_MODULE and enter `POTENTIAL`.
2. Specify which substance or solution database to use. Any substance or solution database can be used that has a gaseous mixture phase, metals (or alloys), and solids such as metaloxides, sulphides, sulphates, carbonates, silicates, nitrides, and nitrates (stoichiometric or solution phases).
3. Specify the matrix element (a metal) and the two gaseous species that define you metal-gas interaction system. The names of these components must be available in the database you are using.
4. Set the temperature (in Kelvin). (The pressure is always 1 bar.)

A potential diagram with the activities of the two gaseous species as mapping variables is calculated. These mapping variables are also set as the axis variables in the plotted diagram.



The following is an example diagram (from example 35 in the *Console Mode Examples*).



A POLY3 file is also automatically saved in the current working directory with the default name POT.POLY3.

5. When the diagram is plotted, it opens the POST module where you can modify the plotted diagram in any way you like.

Calculating a Potential Diagram with Different Pressure

It is possible to modify both the calculation and the plotted diagram that the POTENTIAL module generates in the POLY and POST modules. You can do this by opening a POLY3-file with the results from a POTENTIAL module calculation in either POLY or POST. You can modify the calculation in the same way that you can modify any ordinary mapping calculation or phase diagram. For example, this is useful for calculating a potential diagram at a pressure other than 1 bar.

► ["POLY Module Commands" on page 131](#)

You must have calculated a potential diagram already, and have the saved POLY3-file available.

1. Use GOTO_MODULE and enter POLY.
2. Use READ followed by the name of the POLY3 file that contains the results of the

potential diagram calculation that you want to modify.



A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

3. This opens the workspace file and loads the previous settings and results. The activities of the two gaseous species is now part of the conditions, and these conditions are set as the mapping variables.
4. Use `SET_CONDITION` to specify the pressure under which you want the potential diagram to be calculated. For example, to set the pressure to 1000 bar, enter:

```
SET_CONDITION P=1e8
```

5. Use `COMPUTE_EQUILIBRIUM` to compute the initial equilibrium.

You may also want to use `ADD_INITIAL_EQUILIBRIUM` to calculate some additional equilibria that the mapping calculations are based on.

6. Use `MAP` to perform the mapping calculations.
7. Use `GOTO_MODULE` and enter `POST` to set conditions for visualization and to plot the diagram.

Scheil Simulations

In this section:

| | |
|------------------------------------------------------------|----|
| About the Scheil-Gulliver Solidification Simulations | 72 |
| Simulating a Scheil Solidification Process | 75 |
| Scheil Module State Variables | 78 |
| Scheil Module Frequently Asked Questions | 79 |

About the Scheil-Gulliver Solidification Simulations

Thermo-Calc is often used to perform equilibrium calculations, but some non-equilibrium transformations or partial-equilibrium transformations can also be simulated.

A well known example of a non-equilibrium calculation is the *Scheil-Gulliver solidification simulation*.

Classic Scheil Simulation

For the *Scheil-Gulliver solidification simulation*, generally referred to in Thermo-Calc as a classic *Scheil simulation*, the following assumptions are made.

- Diffusion in the liquid phase is assumed to be very fast, that is, infinitely fast.
- Diffusion in the solid phases is so slow that it can be ignored, that is, diffusion is assumed to be zero.
- The liquid/solid interface is in thermodynamic equilibrium.

In this Scheil simulation the temperature is decreased step-by-step. When the temperature drops below the liquidus temperature the equilibrium amount and composition of solid and liquid phase is calculated. The solid phase is removed from the system and only the amount and composition of the liquid phase is used for the next calculation step at a lower temperature. Again, the equilibrium amount and composition of solid and liquid phase is calculated and again the solid phase is removed from the system for the next step. This procedure is repeated until the last liquid disappears.

This calculation procedure is equivalent to assuming that there is no diffusion in the solid phase and infinitely fast diffusion of all elements in the liquid phase. It has been shown to be a good approximation of the solidification of most alloys such as Ni-superalloys, Cu alloys, Al alloys, Mg alloys, and others. However, for steels it fails badly. The reason is that carbon is one of the most important alloying elements in steels and it dissolves interstitially. Carbon therefore has very fast diffusion rates. The assumption of no diffusion in the solid phase during solidification is thus not correct for carbon at most industrial or lab-scale solidification rates.

For this reason a variant of the Scheil simulation was developed and implemented in Thermo-Calc, where one or more elements can be defined as *fast diffusers*.

Scheil Simulation with a Fast Diffuser Element

The *Scheil simulation with fast diffuser* model in Thermo-Calc takes into account the concept of the *fast diffuser*. Typically, C is defined as a fast diffuser, but also other elements such as N, O, or others can also be defined.



Fast diffuser does not quite define this since diffusion is not actually simulated. It is simply assumed that the “fast diffusers” distribute throughout the solid and liquid phase according to thermodynamic equilibrium. This corresponds to *infinitely fast diffusion*.

For the *Scheil simulation with fast diffuser* the following assumptions are made.

- Diffusion of all elements in the liquid phase is infinitely fast.
- Diffusion of all elements in the solid phases, except the ones defined as “fast diffusers”, is zero.
- Diffusion of the elements defined as “fast diffusers” is infinitely fast in the solid phase.
- The liquid/solid interface is in thermodynamic equilibrium.

The classic Scheil simulation and Scheil simulation with fast diffuser models can be considered *thermodynamic* models. There are clear limitations as a certain amount of back diffusion always takes place in the solid phase at real solidification. For this reason, a more sophisticated kinetic model, the *Scheil simulation with back diffusion* is also available.

Scheil Simulation with Back Diffusion

The *Scheil simulation with back diffusion* kinetic model quantitatively takes into account the real back diffusion of all elements in the primary solid phase (typically the FCC or BCC phase). This model requires the use of both a thermodynamic and mobility database. The calculation also requires the cooling rate to be specified; a fast cooling rate allows for less time for back diffusion and the simulation result is similar to the classic Scheil-Gulliver solidification simulation. A very slow cooling rate allows for almost complete back diffusion, the solidification simulation is then close to an equilibrium calculation. It also requires that the size of the solidification domain is specified. In most cases this domain size corresponds to the secondary arm spacing, as this is where typically the liquid is trapped during solidification.



The secondary arm spacing also depends on the cooling rate. For this reason a simple empirical relation between cooling rate and secondary arm spacing is predefined in Thermo-Calc.

For the Scheil simulation with back diffusion the following assumptions are made.

-
- Diffusion of all elements in the liquid phase is infinitely fast.
 - Diffusion of all elements in the primary solid phase are quantitatively calculated using mobility data, a cooling rate and a domain size (typically this is the secondary arm spacing).
 - The liquid/solid interface is in thermodynamic equilibrium.

Summary

The variants of the Scheil-Gulliver solidification simulation (classic Scheil simulation, Scheil with a fast diffuser element, and Scheil with back diffusion) are set up in either the SCHEIL module in Console Mode or the Scheil Calculator in Graphical Mode.



The Scheil with back diffusion feature is only available for systems with diffusion data, i.e. it requires the use of a mobility database.

The Scheil calculation allows the calculation of:

- The solidification range of an alloy.
- Depression of the solidus temperature due to segregation.
- Composition of the last liquid to disappear in segregation pockets.
- Phases formed on final solidification in segregation pockets.
- The composition gradient in the primary solid phase(s) (segregation profile).

After you enter the module and use the ["START_WIZARD" on page 250](#) command, you are prompted to answer a series of questions about which database to use, what the major element is, and the amount of alloying elements. Thermo-Calc then displays a property diagram showing how the fraction of solid phase varies with temperature (in Celsius). You can then plot diagrams using other variables you are interested in. To plot diagrams, you add a new simulation or open a file with the results of a previous simulation. For example, you might be interested in plotting the fraction of remaining liquid against temperature, the fraction of each solid phase or the total of solid phases against temperature, the microsegregation in each solid phase, or the latent heat evolution against temperature.

SCHEIL MODULE EXAMPLES

See the following Thermo-Calc Console Mode examples:



[tcex15 and tcex30](#) to simulate non-equilibrium transformations without considering fast-diffusion elements.



[tcex48](#) to simulate partial-equilibrium transformation with fast-diffusion elements taken into consideration. This example also shows how you can perform lever-rule calculations (full-equilibrium transformations).



[tcex54](#) for a solidification simulation of a Al-2.1Cu-1Si alloy where back diffusion in the primary phase is included.

SCHEIL AND THE DIFFUSION MODULE (DICTRA)



If you also have a license for the Diffusion Module (DICTRA), you can import a previously calculated Scheil segregation profile into the software using the command `INPUT_SCHEIL_PROFILE`. Press F1 to search the online help.

Simulating a Scheil Solidification Process



["SCHEIL Module Commands" on page 246](#)



["About the Scheil-Gulliver Solidification Simulations " on page 72](#)

Simulating a Scheil-Gulliver solidification process involves calculating the liquid composition of a higher-order multicomponent system at each step of a cooling process, and resetting the liquid composition as the composition of the entire system (after having removed all amount of solid phase).



The step-by-step instructions below are intended as a simple example of setting up a calculation using the wizard. You can also use the macros available and briefly described in ["Examples of Scheil-Gulliver Calculations" on page 434](#).



The following does not include any prompts related to using back diffusion. See ["START_WIZARD" on page 250](#) for additional details about when this is enabled with the ["USE_BACK_DIFFUSION" on page 253](#) command.

1. At the prompt type `GOTO_MODULE SCHEIL`.
2. Type `START-WIZARD` and press <Enter>.
3. Specify which `Database` to use. Type `?` for a list of available databases based on your license.

-
- Type `FEDEMO` for this example.
4. Specify the `Major element or alloy` in your system. For example, enter `Fe` (steel/Fe-alloy), `Al` (Al-based alloy), or `Ni` (Ni-based super alloy).
 - Type `Fe` for this example.
 5. Set whether to specify the `Composition input in mass (weight) percent` (the default) or in `Mole percent`. Press `<Enter>` to keep the default for mass percent or type `N` to use mole percent.
 - Keep the default for this example (press `<Enter>`).
 6. Specify the name of the `1st alloying element`. You can directly specify mass or mole percent after the name. If this is not specified, then you are prompted to enter it separately.
 - Type `Cr 5` for this example.
 7. Specify the other alloying elements in the same way as you specify the first.
 - Type `c 1` for this example.
 8. After you have specified your last alloying element, press `<Enter>`. This ends the process of defining the bulk composition of the alloy system.



You can also specify all the alloying elements and their corresponding compositions on the same line when you are prompted to specify your first alloying element. As a general example, you can enter `Cr 5 Ni 1 Mo 0.5 C 0.01 N 0.02`.

- Press `<Enter>` for this example.
9. Specify the starting `Temperature (C)` in Celsius. The default is `2000`.

This value should be sufficiently high so that the solidification simulation starts with the alloy system in the liquid single-phase region.

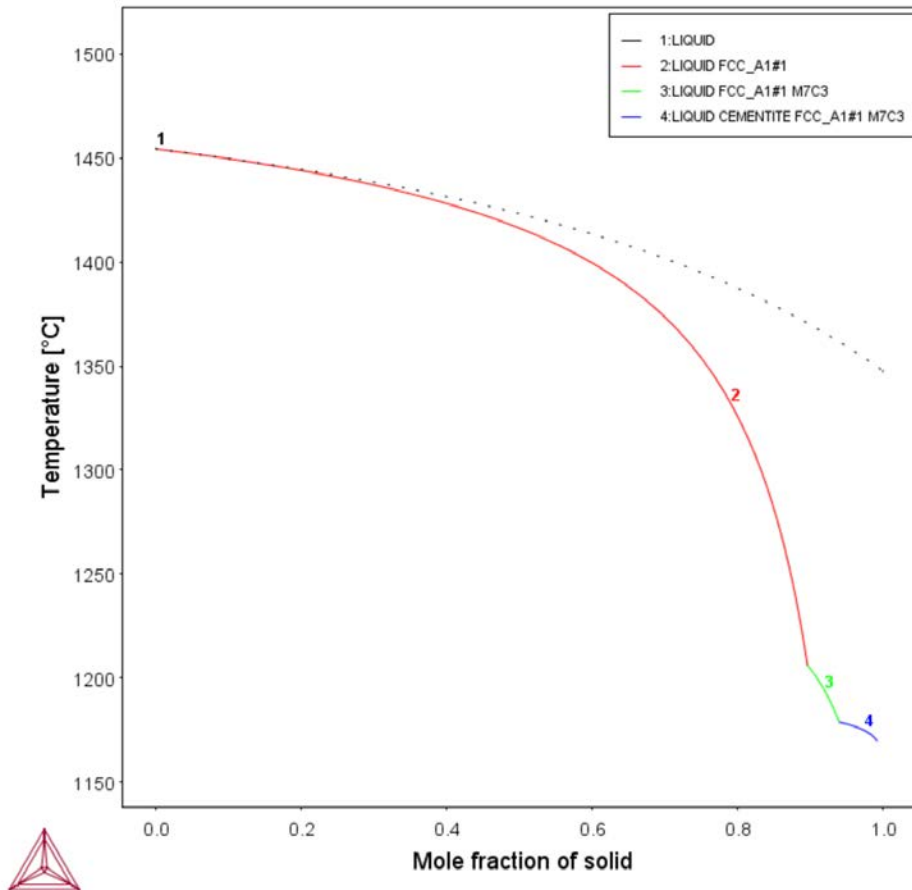
 - Keep the default for this example (press `<Enter>`).
 10. At the `Reject phase(s)` prompt enter the name of the phases to reject or press `<Enter>` for the default `NONE`.
 - Keep the default `s` for this example (press `<Enter>`).
 11. At the `Restore phase(s)` prompt you may want to restore a phase that you rejected when you ran the simulation earlier, or you may want to restore a phase that is rejected by default in your database. Enter the name of the phases to restore or
-

press <Enter> for the default `NONE`.

- Keep the default for this example (press <Enter>).
12. When prompted `OK?` type `N` to go back to reconsider which phases to reject or restore. Type `Y` to continue. The thermodynamic data about the alloy system you defined is retrieved from the database.
 - Keep the default for this example (press <Enter>).
 13. At the `Should any phase have a miscibility gap check` prompt, press <Enter> for the default `N` or type `Y` then specify the `Phase with miscibility gap`.
 - For this example, type `Y` then enter `FCCas` the phase with miscibility gap.
 14. If you answer `Y` to the miscibility gap check, then next enter the following for `Major constituent(s) for sublattice 1` and `Major constituent(s) for sublattice 2`.
 - Enter `Cr` for sublattice 1 and `C` for sublattice 2 in this example. Then at the `Phase with miscibility gap` prompt press <Enter>. The system responds with `LIQUID PHASE NAME: LIQUID`.
 15. Specify the names of any `Fast-diffusing components`. Press <Enter> for `NONE` or type all the names on the same line then press <Enter>.
 - Keep the default for this example (press <Enter>).

The Scheil-Gulliver solidification simulation runs, and the diagram *Temperature versus Mole Fraction of Solid* is plotted in the Console Results window.

2019.11.12.07.27.56
 FEDEMO: C, CR, FE
 T=1727.57, W(CR)=5E-2, W(C)=1E-2, P=1E5, N=1



Scheil Module State Variables

Post processing is done the same way as POLY-3: specific variables for plotting in the Scheil Module are listed.

► ["POLY Module Commands" on page 131](#)

The variables can be plotted along the X- and Y-axes. In the table, *ph* is an abbreviation of *phase*, and *el* is an abbreviation of *element*. Use the abbreviations of the variables when you specify what the X- and Y-axes represent in a diagram.

| Abbreviation | State variable |
|--------------|------------------------------|
| T | Temperature in Celsius |
| NL/BL | Mole/mass fraction of liquid |

| Abbreviation | State variable |
|---------------|--------------------------------------------|
| NS/BS | Mole/mass fraction of all solid phases |
| NS(ph)/BS(ph) | Mole/mass fraction of a solid phase |
| W(ph,el) | Weight fraction of an element in a phase |
| X(ph,el) | Mole fraction of an element in a phase |
| Y(ph,el) | Site fraction of an element in a phase |
| NN(ph,el) | Distribution of an element in a phases |
| NH/BH | Heat release and Latent heat per mole/gram |
| CP/BCP | Apparent heat capacity per mole/gram |
| NV/NV(ph) | Molar volume of the system or a phase |
| DS/DS(ph) | Average density of the system or a phase |
| BT | Apparent volumetric CTE of the system |

Scheil Module Frequently Asked Questions

HOW CAN I PLOT THE LATENT HEAT EVOLUTION AFTER A SCHEIL SIMULATION?

The total or apparent heat release during the solidification process consists of two parts: one is the so-called latent heat, i.e. heat due to the liquid → solid phase transformation, and the other is the heat related to the specific heat of liquid and solid phases. To examine the heat evolution after a Scheil simulation, one can in Console Mode choose either NH or BH from the list of available plotting quantities to plot both (total or apparent) heat release and latent heat evolution against T, the temperature. This will result in a diagram with two curves, where the upper curve represents the latent heat evolution, whereas the lower curve represents the (total or apparent) heat release. By choosing NH the result is displayed as J/mol, whereas BH gives the result as J/gram. If one wants to plot just a single curve, one has to save the results to an .EXP file and re-plot after editing it.

WHAT IS THE DIFFERENCE BETWEEN HEAT RELEASE AND LATENT HEAT EVOLUTION FOR A SCHEIL SOLIDIFICATION SIMULATION?

The total or apparent heat release during the solidification process consists of two parts: one is the so-called latent heat, i.e. heat due to the liquid → solid phase transformation, and the other is the heat related to the specific heat of liquid and solid phases. To examine the heat evolution after a Scheil simulation, one can in Console Mode choose either NH or BH from

the list of available plotting quantities to plot both (total or apparent) heat release and latent heat evolution against T , the temperature. This will result in a diagram with two curves, where the upper curve represents the latent heat evolution, whereas the lower curve represents the (total or apparent) heat release. By choosing NH the result is displayed as J/mol, whereas BH gives the result as J/gram. If one wants to plot just a single curve, one has to save the results to an .EXP file and re-plot after editing it.

WHY ARE THERE TWO CURVES WHEN PLOTTING HEAT EVOLUTION AFTER A SCHEIL SIMULATION?

The total or apparent heat release during the solidification process consists of two parts: one is the so-called latent heat, i.e. heat due to the liquid \rightarrow solid phase transformation, and the other is the heat related to the specific heat of liquid and solid phases. To examine the heat evolution after a Scheil simulation, one can in Console Mode choose either NH or BH from the list of available plotting quantities to plot both (total or apparent) heat release and latent heat evolution against T , the temperature. This will result in a diagram with two curves, where the upper curve represents the latent heat evolution, whereas the lower curve represents the (total or apparent) heat release. By choosing NH the result is displayed as J/mol, whereas BH gives the result as J/gram. If one wants to plot just a single curve, one has to save the results to an .EXP file and re-plot after editing it.

Aqueous Solutions and Pourbaix Diagrams

In this section:

| | |
|--------------------------------------------------------|----|
| About Aqueous Solutions and the Pourbaix Diagram | 82 |
| Calculating a Pourbaix Diagram | 84 |
| Plotting More Pourbaix Diagrams | 86 |
| Stepping Calculations in an Aqueous Solution | 88 |
| POURBAIX_DIAGRAM Module | 89 |

About Aqueous Solutions and the Pourbaix Diagram



This command or module is not available with GES6.



GES6 is a re-write and new implementation of the Gibbs Energy System module of Thermo-Calc and it is the default engine. The previous version, GES5, is still available and will continue to work in the background of the program where necessary. The main purpose of GES6 is to support faster development of new features. However, not all GES5 functionality is implemented in GES6. In such cases (except for optimization, PARROT and the POURBAIX module), GES6 falls back silently and uses functionality from GES5 in the background.

Heterogeneous equilibrium calculations involving aqueous solutions are not different from other equilibrium calculations, but the setup of the equilibrium conditions and the reference states of the system is more complex. For example, the pH and Eh values of the aqueous solution phase are normally complex functions of bulk composition, temperature and pressure conditions.

For some simple systems, thermodynamic approximations of pH-Eh calculations can be used. But Thermo-Calc also has comprehensive thermodynamic models and databases for various non-ideal solution phases. These let you accurately calculate pH and Eh property diagrams (and many other types of property diagrams) in complex aqueous solutions in a variety of conditions.

A Pourbaix diagram is a kind of phase diagram that shows the stability boundaries for a metal-aqueous interaction system. The phase boundaries are shown as a function of pH (acidity) and Eh (standard hydrogen electronic potential). An aqueous solution phase is always present in such a system. At a given pH and Eh, a metal may lose its stability to a soluble or corrosive aqueous solution, or be in equilibrium with either the aqueous solution (insoluble/immune) or with a secondary-phase file that has formed (consisting of oxides, hydroxides, sulphides or other solids). In the latter case, further dissolution of the passive or protective metal is prevented.

A Pourbaix diagram is a pH-Eh phase diagram where the tie-lines are not in the plane. The chemical potentials or activities of two system components (H^+ and EA) are used as mapping variables and the pH and Eh quantities are normally plotted on the X- and Y-axes of the diagram. You can use many other properties as axis variables in various property diagrams for the interaction system at a specific temperature and pressure. The phase relations

between the aqueous solution and various metal forms, oxides, hydroxides, sulphides, sulphates, nitrates, silicates, carbonates and other solids, or gaseous mixtures, are represented as different fields defined by acidity and electric potential.

The POURBAIX module lets you construct Pourbaix diagrams and other types of property diagrams for heterogeneous interaction systems with aqueous solution phases. The compositional definition and variations and the basic solvent and electron components H₂O, H+1 and ZE are automatically determined by the aqueous solution phase in the Pourbaix module.



See Console Mode examples [tcex40](#) and [tcex53](#).

KEY COMPONENTS

These key components are defined as follows:

| Component | Component status | Reference state | Ref-T(K) | Ref-P(Pa) |
|------------------|------------------|---------------------|----------|-----------|
| H ₂ O | ENTERED | AQUEOUS | * | 100000 |
| H+1 | ENTERED | SER | | |
| ZE | ENTERED | REFERENCE_ELECTRODE | * | 100000 |

Besides the aqueous solution phase, your system may also contain a gaseous mixture phase. Other neutral and charged gaseous species may also be constituents. For multicomponent systems there are normally also some interacting solid phases (stoichiometric or solution) as the so-called secondary phases. These are typically the matrix and/or precipitate phases in the alloys of interest.

Some databases have been specially developed for the Pourbaix module's diagram calculations. Such a database contains all necessary phases, i.e., an aqueous solution phase, a gaseous mixture phase, some alloy solid solution phases and some secondary solid phases. Databases developed for the Pourbaix module include *PAQ* (TCS Public Aqueous Solution Database) or *PAQS* (TGG Public Aqueous Solution Database).



If such a dedicated Pourbaix module is not used, then an aqueous solution database such as *TCAQ* (TC Aqueous Solution Database), *AQS* (TGG Aqueous Solution Database), or any user-specified aqueous databases can be used.

This database contains at least the AQUEOUS and REFERENCE_ELECTRODE phases. The aqueous solution database needs to be appended with additional required data and phases,

such as interacting alloy (solid) solution phases and secondary (solid and liquid) phases. Additional data is from one or more databases, such as SSUB/SSOL/TCFE or other substances/solutions databases.

Calculating a Pourbaix Diagram

The POURBAIX module lets you construct Pourbaix diagrams and other types of property diagrams for heterogeneous interaction systems with aqueous solution phases.

When calculating a Pourbaix diagram, you need to have a database with an aqueous solution phase (that is, a phase with water as the dissolving solvent and with aqueous cation/anion and complex species as the dissolved solutes). Due to restrictions of aqueous solution models (SIT, HKF, Pitzer) used in the Thermo-Calc software, the aqueous solution database must be designed in the same Thermo-Calc database format as that used in the PAQ, PAQS, TCAQ and AQS databases for the aqueous solution phase.

Pourbaix diagram calculations are done in the advanced Pourbaix module.

HOW TO CALCULATE A POURBAIX DIAGRAM

1. At the `SYS` prompt, enter `GOTO_MODULE POURBAIX`.
2. At the `Need any instruction on the POURBAIX module?` prompt, press `<Enter>` to skip or enter `y` to learn more.
3. Press `<Enter>` at the prompt `Enforce a PAUSE after plotting when running a MACRO?`.
4. Press `<Enter>` to accept the default `1` to `Start a completely new POURBAIX diagram calculation` or enter `3` to `Open an old file and make another POURBAIX calculation`.

To choose `3`, you must have already done a Pourbaix calculation and have it saved in a `POLY3` file. The new calculation uses the same system definition as the previous calculation, but the other conditions, such as the bulk composition, temperature and pressure, can be modified in the next step.

5. Type `y` or `n` to set whether to `Consider the GAS phase (gaseous mixture phase)` in the calculation.

The gaseous mixture phase should at least contain H₂O, O₂ and H₂. If a GAS phase is not considered, then only the interactions between the aqueous solution phase and various solid phases (alloy phases and secondary phases) are calculated. Such a calculation may not accurately present all the heterogeneous interactions. Some secondary phases are therefore usually needed. Such phases exist in the PAQ or PAQS Public Aqueous Solution Databases. They can also be appended from the SSUB/SSOL/TCFE or other appropriate substances/solutions databases.

6. Type `Y` or `N` to set whether to Use single database (`Y`) or a multiple database (`N`).

If you choose to use a single database, at the Combined Database: /PAQ2/ prompt specify a database that is specially developed for the Pourbaix module's diagram calculations.

If you choose to use a multiple database, then you are prompted to specify an aqueous solution database and to append any additional required data and select necessary phases, such as various interacting alloy (solid) solution phases, and secondary (solid and liquid) phases, for example.

7. Specify all your solutes and the molality of each solute when prompted to do so. This can be done in terms of elements (such as Fe, Ni, Na, Cl, C or S) or arbitrary complex species (such as NaCl, CO₂, CoCl₃, Fe_{0.93}S, NaSO₄-1, or H₂SO₄). You can enter the element/species and the molarity on one line (for an example, NaCl 2.5).



The first letter of the element abbreviation must always be upper case. Any second letters must be lower case. When you have finished your specification, press <Enter> when asked to specify Next solute.

The definition of your system and its initial bulk composition is now presented.

8. Type `Y` to confirm the defined system and its bulk composition.

The thermodynamic data for your system is now retrieved from the database(s) chosen.

9. Answer the questions that you are prompted regarding various parameters of your calculation. You are asked to do any of the following:

- Rejectphase(s) OR Restore phases(s)
- Check for miscibility gaps on any phase (Should any phase have a miscibility gap check?)

-
- Enforce the Global Minimization Technique in calculations?

- Save all functions, variables and tables in POLY3 file?

- Set numerical limits on the calculation

- Confirm defined conditions?

- Accept the default settings for two mapping variables

8. The Pourbaix calculation starts. Answer the question Any missing phase boundary you could possibly think of? Type Y or N to set whether you want to add starting points to the calculation. If you suspect that the calculation has missed some phase boundaries, this may help the program to detect them.

9. Answer questions about how the diagram is plotted and how to save the results of your calculation. You are asked to do any of the following:

- Change the pH/Eh steps for smoother curves?
- Zoom in on a specific region of the diagram
- Change the curve-label option for the diagram
- Add label-texts onto the Pourbaix diagram
- Change the subtitle of the diagram
- Change the axis-texts
- Further refine the diagram in the POST Module
- Print the diagram (save a Hard copy of the diagram)
- Save the X-Y coordinates of curve on a text file
- Modify the diagram
- Calculate and plot another Pourbaix diagram (Any more diagram?)

Plotting More Pourbaix Diagrams

When you have calculated a Pourbaix diagram, you can plot additional diagrams based on the results of the same calculation, but with different axis variables than Ph and Eh.

The variables can be plotted along the X- and Y-axes. Use the abbreviations of the variables when you specify what the X- and Y-axes represent in a diagram. In the table, *AQsp* refers to the name of a specific aqueous species. The asterisk (*) can be used as a wild card character for all such species. If neither *AQsp* nor * is entered in parenthesis, then all species are searched.

You must have plotted a Pourbaix diagram to plot a diagram with other variables than Ph and Eh on the Y-axis and the X-axis. You can either plot such additional diagrams directly after having finished the plotting and saving/printing of a Pourbaix Ph-Eh diagram or by choosing option 2 (Open an old file and plot other property diagrams) when you enter the POURBAIX module and opening a POLY3 workspace file.

ABBREVIATIONS FOR AQUEOUS SOLUTION VARIABLES

| Abbreviation | Variable |
|--------------|------------------------------------------|
| pH | Acidity |
| Eh | Electronic Potential (V) |
| Ah | Electronic Affinity (kJ) |
| Pe | Electronic Activity (log10ACRe) |
| IS | Ionic Strength |
| TM | Total Concentration |
| Aw | Activity of Water |
| Oc | Osmotic Coefficient |
| MF(AQsp) | Mole Fractions of Aqueous Species |
| ML(AQsp) | Molalities of Aqueous Species |
| AI(AQsp) | Activities of Aqueous Species |
| RC(AQsp) | Activity Coefficients of Aqueous Species |

HOW TO PLOT AN AQUEOUS SOLUTION DIAGRAM

1. Type γ when prompted whether to plot any more diagrams, or select option 2 when you enter the POURBAIX module.
2. Specify which variable you want the X-axis to represent. Use the abbreviation specified in the preceding table. When you specify the name of an aqueous species, you can use the asterisk (*) to select all species.
3. Specify which variable you want the Y-axis to represent. The diagram is then automatically plotted.
4. Answer questions about how the diagram is plotted and how to save it. You are asked to do any of the following:
 - a. change the axis-type (linear, logarithmic or inverse) on the X-axis or Y-axis

-
- b. zoom in on a specific region of the diagram
 - c. change the curve-label option for the diagram
 - d. add label-texts onto the Pourbaix diagram
 - e. change the subtitle of the diagram
 - f. change the axis-texts
 - g. refine the diagram in the POST Module
 - h. print the diagram (save a hard copy)
 - i. save the X-Y coordinates of curve on a text file
 - j. modify the plotted diagram
 - k. calculate and plot another aqueous solution diagram

Stepping Calculations in an Aqueous Solution



Performing the stepping calculation overwrites all the previous settings and stepping results on the POLY3-file. To avoid this, use ["SAVE WORKSPACES" on page 176](#) to create a new workspace.

When you have calculated a Pourbaix diagram, you can use the saved results of the calculation (the POLY3 file), and make a property diagram based on stepping calculation.

Since the program normally sets the calculated initial equilibrium point as the starting point, the minimum value for the stepping variable must be specified as smaller or equal to the specific initial condition, and the maximum value as larger or equal to that condition. If pH is set as the stepping variable, the program automatically calculates the equilibrium constant in logarithmic ($\log_{10}K_a$) of the electrolysis reaction $\text{H}_2\text{O (water)} = \text{H}^+ + \text{OH}^-$ for the real aqueous solution under the current temperature-pressure-composition conditions, and thus this constant $\log_{10}K_a$ value is considered as the highest pH in specifying the maximum value along stepping. Subsequently, confirm or modify an increment factor with a default value; for pressure and mole of a component, specify the step in logarithmic ($\log_{10}P$ or $\log_{10}N$).

STATE VARIABLE ABBREVIATIONS

You can use any of these state variables as a stepping variable.

| State variable | Abbreviation |
|---------------------------------------------------------------------------------------|---------------------------------|
| Temperature (K) | T |
| Pressure (bar) | P |
| Acidity | pH |
| Electronic potential (V) | Eh |
| Mole number of a dissolving component (such as Fe, Na, Cl, or NaCl) in 1 kg of water. | N(Comp) (for example, N(Fe)) |

HOW TO DO A STEPPING CALCULATION

You must have plotted a Pourbaix diagram before making a stepping calculation on an aqueous solution.

1. Use GOTO_MODULE POURBAIX to enter the POURBAIX module.
2. Type 4 to open an old file and make another STEPPING calculation.
3. Choose which POLY3 file to load.
4. Specify the conditions of the calculation by answering the questions that follows.

The system definition is the same as in the previous Pourbaix calculation, but you can modify conditions such as bulk composition, temperature and pressure, and change some component definitions if necessary.

5. Specify which variable to use as the stepping variable (see the preceding table), its minimum and maximum value, and the length of each incremental step.

The settings and stepping results are written to the opened POLY3 file, and a first default property diagram is plotted.

POURBAIX_DIAGRAM Module



This command or module is not available with GES6.



GES6 is a re-write and new implementation of the Gibbs Energy System module of Thermo-Calc and it is the default engine. The previous version, GES5, is still available and will continue to work in the background of the program where necessary. The main purpose of GES6 is to support faster development of new features. However, not all GES5 functionality is implemented in GES6. In such cases (except for optimization, PARROT and the POURBAIX module), GES6 falls back silently and uses functionality from GES5 in the background.

Getting started with the Pourbaix module

After you enter the POURBAIX_DIAGRAM module, you are asked if you want to have step-by-step instructions to help walk you through the module.

```
Need any instruction on the Pourbaix module? /N/: Y
```

If you answer `y` a series of notes are displayed. The following is a more comprehensive summary of these same notes.

What is a Pourbaix diagram?

The Pourbaix diagram is a calculated equilibrium phase diagram mapped and plotted with the independently-varied electropotential (E_h , as defined with regard to the standard hydrogen electrode as its reference) and acidity (pH), that represents all the equilibrated phase boundaries among aqueous solution, gaseous mixture, and various primary and secondary solids (modeled as either complex solution or simple stoichiometric phases) in a certain multicomponent heterogeneous interaction system, under a defined T-P condition and a specific initial bulk composition (which is, by default, always set as 1 kg of water dissolving a specified amount of metals/alloys and other acids/alkalines/salts).

What database should I use?

At least one database is required that contains an aqueous solution phase (with thermodynamic data for water and various aqueous solutes), that shall be selected from TCAQ (PAQ) or AQS (PAQS) [which use the SIT Model or the Complete Revised HKF Model, respectively] within the Thermo-Calc databases.

Choosing a custom aqueous solution database

You can also use a custom database but it must be in the Thermo-Calc TDB format. Due to the restrictions of aqueous solution models used within Thermo-Calc, such a database must be designed in the same format as in the default TCAQ (PAQ2) for aqueous solution phases. Among other things, keep the following requirements in mind:

The ELECTRON is defined as a special element (ZE) and as the only constituent in its reference phase REFERENCE_ELECTRODE (for determining the electro-potential that is defined as E_h with the standard hydrogen electrode as the reference), but it is not defined as an aqueous species;

The vacancy (VA) is unnecessary for AQUEOUS solution phase and it should be avoided in the definition of phase-constituents in the AQUEOUS phase;

The AQUEOUS solution phase should always be defined as a constitutional solution phase, implying that all the aqueous solution species must be included in a single site, rather than in two or multiple sublattices.

Beside the AQUEOUS solution phase, there shall exist a GAS mixture phase containing at least H₂O, O₂ and H₂; and for multicomponent systems, normally there shall also contain some solid (stoichiometric or solution) phases. Of course, if desired, you could also choose to calculate and generate a Pourbaix diagram without considering the GAS mixture phase entirely; however, such a plot is not really a complete Pourbaix diagram, due to the fact that thermodynamically-stable phase boundaries between the AQUEOUS solution phase and GAS mixture phase will then not be calculated at all!

All the required thermodynamic data for calculations of Pourbaix diagrams or other diagrams must be retrieved either from one (Single) database which consists of an AQUEOUS solution phase, a Gaseous mixture phase, a REF_ELECTRODE phase, and some SOLID phases (being solutions and/or stoichiometric compounds; for primary metals/alloys and for secondary products formed from heterogeneous chemical/electrochemical interactions, or from several (Multiple) databases that respectively contain various solutions/compounds (as listed above).

Such databases suitable for calculations of aqueous-bearing heterogeneous interaction systems can be those default-prompted ones [i.e., in the Single-Database case, the PAQ or PAQS; and in the Multiple-Database case, the PAQ2 or as primarily-switched database, plus the SSUBx as firstly-appended one and the SSOLx as secondly-appended one if it is necessary; even more databases can be appended). Of course, you could also choose to append required data from other appropriate databases (such as TCFE, TCSLD, TCNI/TTNi, TCAL/TTAl, TCMG/TTMg, TTZr, TCMP, SLAG, etc.) for Gaseous mixture phase and for various solid solution and stoichiometric compound phases. Furthermore, an experienced user can also utilize his/her own USER-specified databases in various cases.

The advanced POURBAIX module is designed so that it requires you to just answer some necessary questions, rather than to go through the other Console Mode modules (i.e., TDB, GES5, POLY3 and POST) although you still enter commands at the prompts. Beside the

default plotted Pourbaix diagram, it also allows the user to easily and quickly plot many different properties of the system, stable phases and aqueous species, varied along the calculated phase boundaries for the same defined heterogeneous interaction system. Moreover, it permits the user to directly change some plotting settings and manipulate all kinds of plotted diagrams.

The current advanced POURBAIX-Module has been extended so that it is additionally able to directly perform a normal STEPPING calculation (varied with a specified independent variable) and to easily generate various types of property diagrams, for the same heterogeneous interaction system that has been defined in a previous POURBAIX or TDB-GE55-POLY3-POST calculation.

Copy and Rename the POLY3 file

At the end of a Pourbaix module calculation, a new POLY3 file is automatically saved.



A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.



If you are using a POLY3 file more than once (as is done in the extended examples), it is recommended that you copy and rename the previously-generated POLY3 file. This is so that the required POLY3 file structure and Pourbaix results are not lost. Do this outside of Thermo-Calc i.e. do not save from within Thermo-Calc.



The reason you do not save from within Thermo-Calc is because of how the file is saved. When the command sequence (GO POLY3>SAVE <FILE NAME>.POLY3>Y) is used, the POLY3 workspace of the POURBAIX calculation results in the POLY3 module monitor and all the initial equilibrium points and the mapping/stepping calculation results are lost as well as parts of the POLY3 file structure (e.g., some definitions of the previously defined POURBAIX-type calculation system).

Enforce a Pause

After the initial set of information is displayed, you are asked:

```
Enforce a PAUSE after plotting when running a MACRO? /N/
```

-
- If you choose `Y` a pause is always enforced after each diagram is plotted;
 - If you choose `N`, all the command-lines (answers) for the session continue without stopping or until the `SET_INTERACTIVE_MODE` line in the macro file is reached.

Whenever running a Thermo-Calc macro (TCM) file, you may want to pause after a specific diagram is plotted on screen. This gives you the flexibility to:

- Print it (of EMF/PS format) to a printer
- Convert it (of EMF format) to (PDF) graphical files;
- Save it as an EMF graphical file;
- Dump it as a PNG or BMP graphical file;
- Set background colour for the current diagram
- You can also set the default font/size and change plot layers for sequential plots.

Pourbaix Main Options

If you answer `Y` to the Pause prompt above, these options are displayed:

1. Start a completely new Pourbaix diagram calculation.
2. Open an old file and plot other property diagrams.
3. Open an old file and make another Pourbaix calculation.
4. Open an old file and make another stepping calculation.



["POURBAIX_DIAGRAM Commands for Options 1 to 4" on page 450](#)

Tabulation Reactions

In this section:

| | |
|---------------------------------------------------------------------|----|
| About the Tabulation Reaction Module | 95 |
| Tabulating a Reaction | 96 |
| Tabulating a Substance or Solution Phase at Fixed Composition | 97 |

About the Tabulation Reaction Module

The TABULATION_REACTION (TAB) module can be used to tabulate thermodynamic functions of any type of substance, stoichiometric phase or solution phase, or reaction. The module can tabulate thermodynamic functions of pure stoichiometric phases or solution phases at fixed composition, as well as various kinds of partial derivatives for a pure stoichiometric phase or solution phase at a given composition.

The TAB module begins by evaluating the most stable species of a substance in either a homogeneous state or in a reaction. Results are presented in a table or plotted as a graph.

▶ ["Tabulating a Reaction" on the next page](#)

A reaction tabulation presents you with the following properties, on rows representing different temperature levels:

- Heat capacity change / ΔC_p (Joule/K) in column 2.
- Enthalpy change / ΔH (Joule) in column 3.
- Entropy change / ΔS (Joule/K) in column 4.
- Gibbs energy change / ΔG (Joule) in column 5.

In the case of a tabulation of a substance or solution phase at a fixed composition, the properties presented are the heat capacity, enthalpy, entropy and Gibbs energy, rather than the degree of change in those properties.

▶ ["Tabulating a Substance or Solution Phase at Fixed Composition" on page 97](#)

You can add a 6th column to the table that shows the values of a property or user-defined function of your choice.

```

*****
  T      Delta-Cp      Delta-H      Delta-S      Delta-G
  (K)    (Joule/K)    (Joule)    (Joule/K)    (Joule)
*****
298.15 -4.44006E+01 -9.18800E+04 -1.98115E+02 -3.28120E+04
300.00 -4.43267E+01 -9.19621E+04 -1.98389E+02 -3.24452E+04
400.00 -3.92294E+01 -9.61533E+04 -2.10482E+02 -1.19604E+04
500.00 -3.34122E+01 -9.97861E+04 -2.18613E+02 9.52022E+03
600.00 -2.77768E+01 -1.02842E+05 -2.24200E+02 3.16779E+04
700.00 -2.26324E+01 -1.05358E+05 -2.28088E+02 5.43040E+04
800.00 -1.81080E+01 -1.07390E+05 -2.30808E+02 7.72568E+04
900.00 -1.41889E+01 -1.09000E+05 -2.32710E+02 1.00438E+05
1000.00 -1.08095E+01 -1.10245E+05 -2.34025E+02 1.23779E+05
1100.00 -7.77802E+00 -1.11169E+05 -2.34908E+02 1.47229E+05
1200.00 -5.07556E+00 -1.11807E+05 -2.35464E+02 1.70750E+05
1300.00 -2.93467E+00 -1.12203E+05 -2.35782E+02 1.94314E+05
1400.00 -1.19414E+00 -1.12407E+05 -2.35934E+02 2.17901E+05
1500.00 2.55400E-01 -1.12452E+05 -2.35966E+02 2.41497E+05
1600.00 1.49022E+00 -1.12363E+05 -2.35909E+02 2.65091E+05
1700.00 2.56484E+00 -1.12159E+05 -2.35785E+02 2.88676E+05
1800.00 3.51909E+00 -1.11854E+05 -2.35611E+02 3.12246E+05
1900.00 4.38259E+00 -1.11458E+05 -2.35397E+02 3.35797E+05
2000.00 5.17775E+00 -1.10980E+05 -2.35152E+02 3.59325E+05

```

Tabulating a Reaction

A tabulation of a given chemical reaction provides you with data about the rate of change of the standard tabulation properties at various levels of temperature. You can also add a column for a property of your choice to the table.

1. Use GOTO_MODULE TAB to enter the TAB module.
2. If you want to add one thermodynamic functions to the tabulation calculation, which is present in a sixth column in the table, use ENTER_FUNCTION.

You are prompted to enter the name of the column that is given at its head, and the function itself. The following state variables can be used to define the function: G, H, S, T, P, V and H298.

3. Use TABULATE_REACTION followed by a formula that specifies of the reacting species and products to perform the tabulation calculation. The name of the elements must be entered in upper case letters only. Terminate the chemical reaction with a semi-colon. For example, you can enter:

```
TABULATE_REACTION 3H2+N2=2N1H3;
```

Elements that are designated with a single letter must be followed by a stoichiometry factor, even if this factor is 1. `Co` hence be interpreted as Cobalt rather than as carbon monoxide. Carbon monoxide is entered as `C1O1` or `O1C1`.

4. Set the pressure, the range of temperature that you want the tabulation to cover, and change in temperature between each row in the table. You can also specify if you want to output the calculation results to an EXP-file and whether you want any graphical output, and if so, which column you want to be plotted against temperature.

The tabulation calculation is performed and you are given a table that shows the various properties at each temperature level within the range defined.

If you have chosen to receive graphical output, then the Console Results window presents a graph that plots the column of you chose (on the Y-axis) against temperature (on the X-axis). When this graph is plotted, you are now in the POST module, where you can modify the graph in various ways.

Tabulating a Substance or Solution Phase at Fixed Composition

A tabulation of a substance or solution phase at fixed composition provides you with data about the standard tabulation properties at various levels of temperature for a given chemical reaction. You can also add one extra property column of your choice to the table.



It is important to have already defined the system and retrieved thermodynamic data from a database before using the TAB command.

1. Use `GOTO_MODULE TAB` to enter the TAB module.
2. Use `SWITCH_DATABASE` to switch to a database that contains solution-based data, such as TCFE for example.



You cannot use the default SSUB database when tabulating solution phases at a fixed composition.

3. If you want to add one thermodynamic function to the tabulation calculation, which is present in a sixth column in the table, use `ENTER_FUNCTION`.

You are prompted to specify the column header and the function itself. The following state variables can be used to define the function: G, H, S, T, P, V and H298.

-
4. Use TABULATE_SUBSTANCE followed by the name of the substance or solution phase to perform the tabulation calculation.
 5. Set the pressure, the range of temperature that you want the tabulation to cover, and change in temperature between each row in the table. You can also specify if you want to output the calculation results to an EXP-file and whether you want any graphical output, and if so, which column you want to be plotted against temperature.

The tabulation calculation is performed and a table shows the various properties at each temperature level within the defined range.

If you have chosen to receive graphical output, then the Console Results window presents a graph that plots the column you chose (on the Y-axis) against temperature (on the X-axis).). When this graph is plotted, you end up in the POST module, where you can modify the graph in other ways.

Results

In this section:

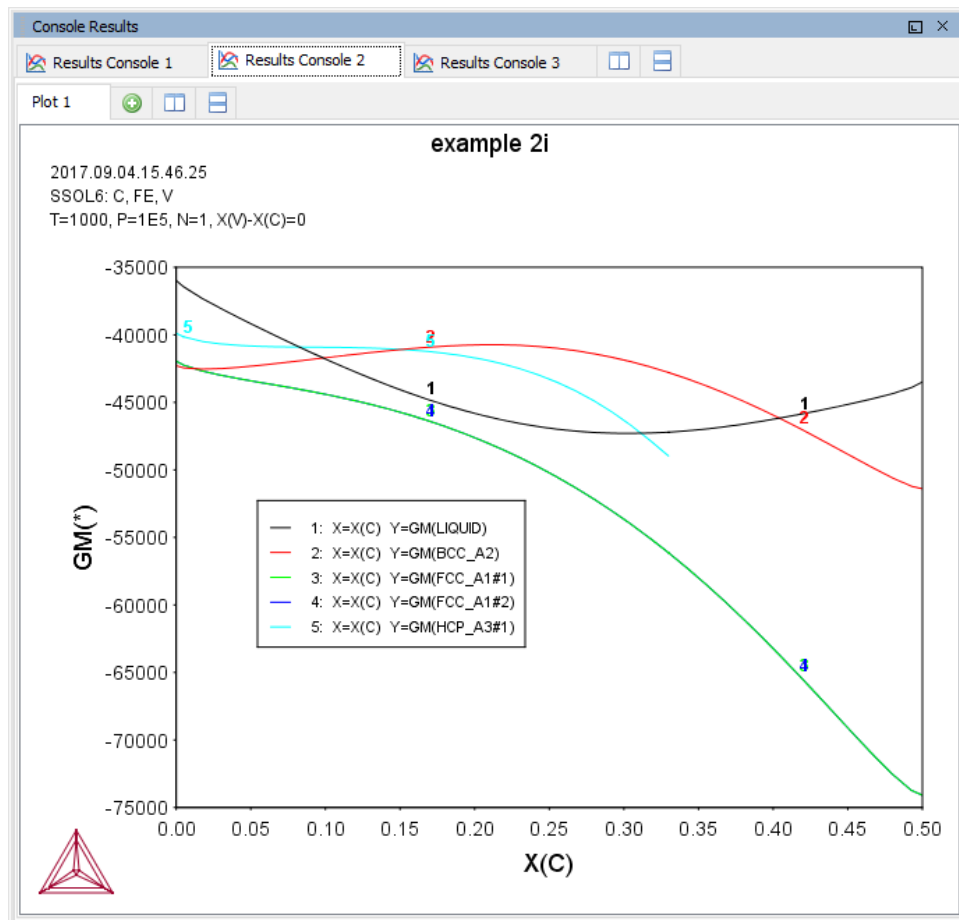
| | |
|------------------------------------------------------|-----|
| Console Mode Results | 100 |
| Using the POST Module | 101 |
| Plotting Diagrams | 101 |
| Saving and Printing the Output in Console Mode | 102 |
| Modifying Diagrams | 106 |
| Loading Saved Diagrams | 108 |
| Working with the Console Mode Output | 108 |

Console Mode Results

The results of a calculation in Thermo-Calc can be plotted by the post-processor module, also called the POST module. The diagram is presented in the Console Results window.

In the POST module, you can define and plot various kinds of diagrams based on a calculation. You can modify diagram type, which variables to plot on each axis and between which minimum and maximum values, append experimental data from an EXP-file, change labels and symbols in the diagram, zoom in on (and out from) a certain region in a diagram, etc.

If you calculate a property or phase diagram in POLY, then you have to open the POST module yourself. If your calculation was performed by a response-driven module such as SCHEIL or POURBAIX, then the plotting of a diagram based your calculation is part of the dialogue of questions and answers you have in that module (but under the hood, the response-driven module is actually utilizing the POST module to get the plotting done).



Using the POST Module

Use the POST module after a ["STEP_WITH_OPTIONS" on page 188](#) or ["MAP" on page 173](#) calculation to generate *graphical* or *tabulated* presentations on screen or into files.

The graphical files are available in different formats (e.g. PS, EMF, PNG, BMP, PDF, JPG, TIF) or data forms (e.g. EXP, TAB and WRL). The graphical output can be phase diagrams, property diagrams, diffusion profiles and other types of plots. The tabulated presentation is into a basic text file (TXT) or a spreadsheet (e.g. an MS Excel file with an extension of .XLS).



The POST module (post-processor) is a submodule to the POLY module and has its own set of commands. The TAB, BIN, TERN, POT, SCHEIL and POURBAIX modules use the POST module features as part of the automatic generation of the plots.

Within the POST module, you can choose any state variable, any derived variable, or any entered symbol (functions or variable) as the X/Y-axis.



["Thermodynamic Variables and Units" on page 381](#)

When a diagram is plotted, appearance parameters for defining a high-standard graph can be further specified, e.g. curve labelling options, diagram titles and subtitles, plot size, axis length, axis types, axis-tic type, tie-line status, automatic or manual scaling and zooming, semi-automatic or manual labelling on phase boundaries and phase regions, graphic formats, text fonts, colours, raster plot, etc.

You can append experimental data onto a plotted diagram. You can also save the coordinates onto a textual file, which can be edited and used as an experimental data file to be merged onto another diagram or as a part of a setup file for PARROT-module assessment.

Phases can be suspended or restored in a plotted diagram. The reference states for components can also be modified for the resulted diagrams. Moreover, you can translate a plotted property diagram (after a stepping calculation) into a tabulated form, such as a simple list on screen or a textual file, and a spreadsheet .

Plotting Diagrams

Plotting a diagram is to graphically represent how several variables (typically two variables) co-vary. Each axis in a property diagram or a phase diagram represents the value of one variable. The default variables represented by the X- and Y-axes are the following:

- If you plot a diagram based on the results of a mapping operation (a phase diagram), then by default the X- and Y-axes represent the mapping axis variables 1 and 2 (set using ["SET_AXIS_VARIABLE" on page 180](#) in POLY).
- If you plot a diagram based on the results of a stepping operation (a property diagram), then by default, the X-axis represents the stepping variable (set using SET_AXIS_VARIABLE) and the Y-axis represents the sum of the mole fractions of all phases (that is, NP(*)).

► ["POLY Module Commands" on page 131](#)

HOW TO PLOT A DIAGRAM

To plot a diagram, you must have already made a stepping or mapping operation in POLY (or in some cases, made a calculation as part of some opening a response-driven module), and you must have entered the POST module.

The POST command is available inside POLY. Use POST to enter the POST module

1. If you want to directly plot your diagram with the default variables represented by the X- and Y-axes, type `PLOT` and press <Enter>. This plots a property or phase diagram with the default variables represented at each axis. If you do not want to plot your diagram with these default variables, go to the next step.
2. Use SET_DIAGRAM_AXIS to set which variables to plot on the X-axis and the Y-axis. For example, if you want to plot a phase diagram with pressure on the Y-axis and temperature on the X-axis, type:

```
SET_DIAGRAM_AXIS X T
SET_DIAGRAM_AXIS Y P
```

3. Use PLOT_DIAGRAM to plot your diagram.

Saving and Printing the Output in Console Mode

► ["Global Settings: Graphical and Console Mode Plotting" on page 47](#)



Output can refer to results in the form of tabulated data in a table or a diagram.



The terms *diagram* and *plot* are interchangeable. The commands in Console Mode generally use the term diagram and in Graphical Mode it is also called a plot (e.g. the Plot Renderer).

Commands to Save and Print Diagrams

Use the following commands to create diagrams, which then display in the **Console Results** window. From this window, you can right-click the diagram and choose **Save as** or **Print**. You can also use the following commands for these actions.

PLOT_DIAGRAM

After you use the SET_PLOT_FORMAT command to define the default graphic device (the printer) you can use a ["PLOT_DIAGRAM" on page 361](#) command to either save the calculation output to a file or display the output in the **Console Results** window.

DUMP_DIAGRAM

["DUMP_DIAGRAM" on page 355](#) is an alternative command used to create output. After a diagram is displayed to the **Console Results** window with the PLOT_DIAGRAM command, you can save (dump) it to a file using this command.

MAKE_EXPERIMENTAL_DATAFILE

Use ["MAKE_EXPERIMENTAL_DATAFILE" on page 360](#) to save all the data about the plotted diagram in an EXP-file. An EXP-file is a plain text file that describes the diagram in the DATAPLOT graphical language. Note that information about the underlying calculations that the diagram is based on is not saved in an EXP-file.

► *DATAPLOT User Guide* included with this documentation set.

PRINT_DIAGRAM

First use PLOT_DIAGRAM to create output that displays in the **Console Results** window. Then after entering the ["PRINT_DIAGRAM" on page 361](#) command, the **Print** window opens where you can choose additional settings for a hard copy of the diagram.

Commands to Save Tables

Tables or tabulated data can be listed in the **Console** window. You then use commands to save the text to different file formats (txt, html, or xls) where you can then print the information.

- ["LIST_DATA_TABLE" on page 358](#): Use this command to output to the screen or to file.
- ["TABULATE" on page 201](#)

Saving Diagrams

You can save the output in a variety of file formats. For JPG and PNG images you can also adjust the image quality.



In Console Mode, the diagram is output to the **Console Results** window after using the PLOT_DIAGRAM command.



In Graphical Mode, the diagram is output to the **Results** window after performing a tree that includes a Plot Renderer.

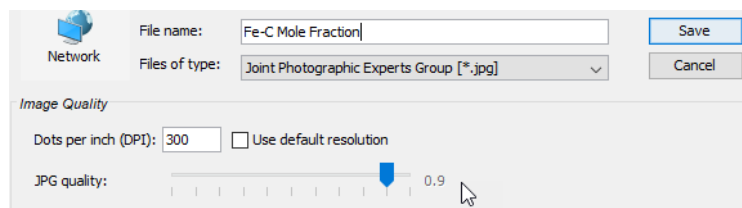
1. In the **Results** window, right-click the diagram and select **Save as**.



In the Graphical Mode **Configuration** window you can also click the **Save Diagram** (or **Save table**) buttons to open the **Save** window.

2. In the **Save** window:

- a. Navigate to where you want to save the diagram.
- b. Enter a **File name**.
- c. From the **Files of type** list choose **png**(the default), **jpg**, **ps**, **pdf**, **gif**, **svg**, or **emf**.
- d. For PNG and JPG files only, under the **Image Quality** section, choose to improve the resolution of the image. For JPG files you can also adjust the file size.
 - To change the resolution of a PNG or JPG image, click to clear the **Use screen resolution** check box. Then enter a numerical value in the **Dots per inch (DPI)** field.
 - For JPEG files, you can also use the slider to choose a number between 0 and 1 for the **JPG quality**. The default is 0.9. The lower the number, the smaller the file.



- e. When you are ready, click **Save**.

Printing Diagrams

In the **Console Results** window, right-click the diagram and choose **Print**. Select additional settings as required on the **Print** window.



Use the ["LIST_DATA_TABLE" on page 358](#) command to save to file and then print the file.

Modifying Diagrams

Modifying a diagram amounts to changing the settings that determine how the POST module presents the calculated results and plots a new diagram. Suppose that you have already plotted a binary phase diagram with the mapping axis variables temperature and mole fraction of one of your components (the Fe component, say) on the X- and Y-axes. If you then want to modify your diagram so that the Y-axis instead represents, say, the mass fraction of Fe rather than the mole fraction, then you use ["SET_DIAGRAM_AXIS" on page 366](#) to set diagram axis Y to $w(Fe)$, and then use ["PLOT_DIAGRAM" on page 361](#).

There are many ways in which you can modify your diagram and how it is presented. Any modification made in the plot settings is taken into account the next time you use PLOT.

EXAMPLE COMMANDS TO USE

The following are some of the modifications you can make.

- Use ["SET_TITLE" on page 375](#) to set add a title or to change an already existing title. The title is displayed above the plotted diagram in the Console Results window.
- Use ["ADD_LABEL_TEXT" on page 352](#) to add a label text that starts at a certain X- and Y-coordinate. If you have plotted a phase diagram, then you can let Thermo-Calc set the label text that specifies the names of the stable phases at that coordinate.
- Use ["SET_AXIS_TYPE" on page 364](#) to set whether the scale of an axis is linear, logarithmic or inverse.
- Use ["SET_DIAGRAM_TYPE" on page 368](#) to plot a triangular diagram with the X-axis on the triangle's base and the Y-axis on the triangle's left side. Such a diagram is often useful if you want to plot the fractions of two components in a ternary diagram.
- Use ["SET_SCALING_STATUS" on page 374](#) to modify the range of values that are displayed on an axis. In effect, you can use it to zoom in or out of the diagram. For example, to set the scale of the X-axis to range from 0 to 0.3, type:

```
SET_SCALING_STATUS X N 0 0.3
```

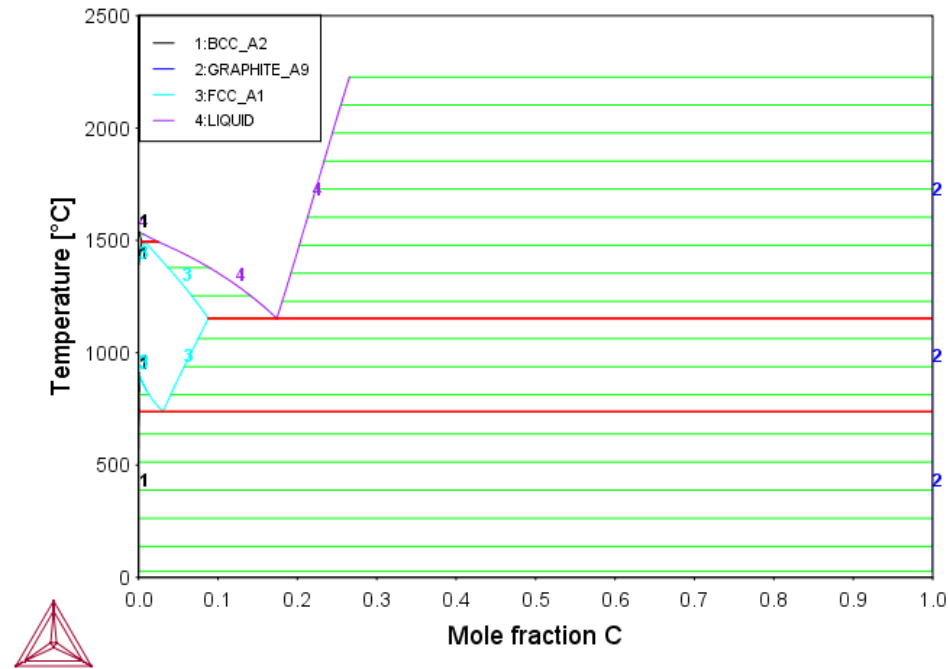
The X specifies which axis to change the scaling on, the N turns off Thermo-Calc's automatic scaling, and 0 and 0.3 specifies the minimum and maximum values on the scale. You can turn on automatic scaling again by setting the second parameter to Y .

- Use ["SET_LABEL_CURVE_OPTION" on page 369](#) to label each set of curves that have

the same stable phases with a certain digit. A legend is also added, where you specify which phases each digit designates.

C FE

2017.09.04.15.39.12
TCBIN: C, FE
P=1E5, N=1



LTEXT vs LATEX COMMANDS FOR LABELS



As of Thermo-Calc 2015a the LTEXT text formatting is replaced by LaTeX. For existing users who may have plots and files that use the LTEXT format, and especially when using Console Mode, the following examples show the command changes from LTEXT and its LaTeX equivalent:

| Symbol or text format | LTEXT | LaTeX |
|----------------------------|---------------------------------------------------------------------|-----------------------------------------------|
| Subscripts in an axis text | S-A-TEXT Y N Mole-fraction Al ^{DO2} O ^{DO3} \$ | S-A-TEXT Y N \latex Mole-fraction Al_ 2O_3 |
| Label with subscript | add .13 .15 n c-ZrO ^{DO2} \$ | add .13 .15 n \latex c-ZrO_2 |
| Greek symbol | ADD .05 .50 N ^GRd\$ | ADD .05 .50 N \latex \delta |

Loading Saved Diagrams

If you have previously saved a diagram in an EXP-file, then you can load and superimpose the diagram on another diagram. Both the following command requires you to specify which prologue and dataset(s) that are loaded from an experimental data file.

Use "[APPEND EXPERIMENTAL DATA](#)" on [page 353](#) to plot selected data from an experimental data file (EXP-file). If you have set the axes of the diagram already, the labels on the diagram are not changed when you plot the additional data from the EXP-file, irrespectively of the data in that file.

Use "[QUICK EXPERIMENTAL PLOT](#)" on [page 362](#) to plot selected data from an experimental data file (EXP-file). If you have set the axes of the diagram already, these settings are overwritten with the axes settings from the EXP-file.

Working with the Console Mode Output

Pause, Resume or Stop Output to the Console Window

In response to a command or a lengthy calculation, Thermo-Calc may display a lot of text in the Console window. Use these keyboard shortcuts to pause, resume or stop a process.

- To pause the text on printing press <Ctrl+S>.
- To resume the printing on screen, press <Ctrl+Q>.
- When Thermo-Calc is performing a stepping or mapping operation, the results are continuously printed in the Console window. To stop the calculation of the current

region of the mapping and stop the output, press <Ctrl-A> (Windows) or <Ctrl-C> (Linux).

Controlling Console Output

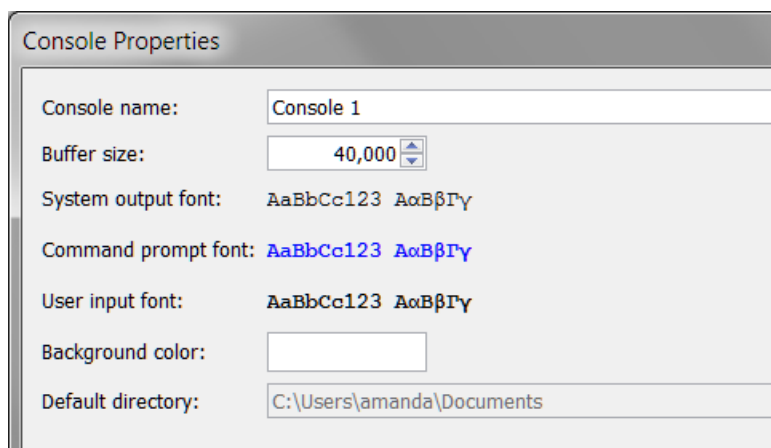
In response to a command or a lengthy calculation, Thermo-Calc may display a lot of text in the Console window. Use these keyboard shortcuts to pause, resume or stop a process.

- To pause the text on printing press <Ctrl+S>.
- To resume the printing on screen, press <Ctrl+Q>.
- When Thermo-Calc is performing a stepping or mapping operation, the results are continuously printed in the Console window. To terminate the calculation of the current region of the mapping and stop the output, press <Ctrl-A> (Windows) or <Ctrl-C> (Linux).

INCREASING THE BUFFER SIZE

In Console Mode, sometimes the output overflows the window text buffer.

1. Right-click the Console tab header in the Console window (if this is the first Console tab, it is labeled **Console 1**).
2. Click **Properties**, and increase the **Buffer size** in the Console Properties window.



Commands by Module

In this section:

| | |
|----------------------------------------------------|-----|
| System Utilities (SYS) Commands | 111 |
| Database (TDB) Module Commands | 122 |
| POLY Module Commands | 131 |
| Gibbs Energy System (GES) Commands | 202 |
| SCHEIL Module Commands | 246 |
| PARROT Module Commands | 255 |
| EDIT_EXPERIMENTS (ED_EXP) Submodule Commands | 285 |
| Tabulation Reaction (TAB) Commands | 321 |
| REACTOR (REACTOR_SIMULATOR) Commands | 342 |
| POST Module Commands | 350 |

System Utilities (SYS) Commands

In this section:

| | |
|----------------------------|-----|
| ABOUT | 112 |
| BACK | 112 |
| CLOSE_FILE | 112 |
| DISPLAY_LICENSE_INFO | 112 |
| EXIT | 113 |
| GOTO_MODULE | 113 |
| HELP (? and ??) | 113 |
| HELP | 113 |
| HP_CALCULATOR | 114 |
| INFORMATION | 114 |
| MACRO_FILE_OPEN | 114 |
| OPEN_FILE | 117 |
| SET_COMMAND_UNITS | 117 |
| SET_ECHO | 118 |
| SET_GES_VERSION | 118 |
| SET_INTERACTIVE | 119 |
| SET_INTERACTIVE_MODE | 119 |
| SET_LOG_FILE | 119 |
| SET_PLOT_ENVIRONMENT | 120 |
| SET_TC_OPTIONS | 120 |
| STOP_ON_ERROR | 121 |

ABOUT

The ABOUT command lists basic information about the development history and ownership of the Thermo-Calc software as well as version information.

BACK

► ["GOTO_MODULE" on the next page.](#)

Use the BACK command to switch control back to the most recent module. Going from the POST module, BACK goes only to the TAB or POLY module (from where the POST module is entered).

CLOSE_FILE

Close an opened text file.

| | |
|--------|----------------------------------------------------------------------------------------------|
| Syntax | CLOSE_FILE |
| Prompt | Unit number: <Unit number> A unit number given in an OPEN_FILE command must be specified. |

DISPLAY_LICENSE_INFO



You can also access this same information from the top menu. Choose **Help → Show License Info.**

Use this command to launch a license diagnostics program implemented in the SYS module. It detects the license information for the Thermo-Calc installations on the current client computer (and on the connected license server), and lists the details, including the current status of available license file and all its included license features for the current installation (s), as well as the Safenet Environment Variables and detailed Local (Client) Information, on screen or into a textual file (*.TXT).

This is useful for a list of license details, and to obtain basic technical support by sending the *.TXT file to support@thermocalc.com. If you are running a network client installation of Thermo-Calc, you can see how many of the client example licenses that are currently checked out and how many of them are left. You can also see which clients computers it is that have checked these client example licenses out.

| | |
|--------|--------------------------------------------------------|
| Syntax | DISPLAY_LICENSE_INFO |
| Prompt | Output to screen or file /Screen/: <Mylicenseinfo.txt> |

| | |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | DISPLAY_LICENSE_INFO |
| | Press <Enter> to display a list of license information or into a *.TXT file under a specific file name which can later on be opened and edited by any basic text editor. |

EXIT

Use the EXIT command to leave the program and return to the operating system. Use a SAVE command before exiting otherwise all data and results are lost (in either the GIBBS, POLY, PARROT or REACTOR module).

GOTO_MODULE

Switch between modules. The name of the module must be typed. To get a list of available modules, press the <Enter> key.

| | |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | GOTO_MODULE |
| Prompt | Module name: <Module name> |
| | If the <Enter> key is pressed without typing a unique module name (or typing a ? mark) it prompts for the MODULE NAME and lists the available modules. |

HELP (? and ??)

Enter ? or ?? to get text help about the current prompt (whether this is the prompt of a module, or a prompt that requests you to specify the value of some parameter).



For some commands and prompts, more detailed help is given when two ?? are entered.

HELP

Lists the available commands or explains a specified command. Specifying a unique command displays an explanation on screen. Typing a command abbreviation that is not unique lists all matching commands. Get the command information by typing a unique abbreviation or the complete command name.

| | |
|--------|----------------------------------------------------------------------------------------------------------|
| Syntax | HELP |
| Prompt | Command: <Command name> |
| | <i>Command name</i> is the name of the command (one of the-module commands) to get help. |
| | If the <Enter> key is pressed without typing a command name, then all the available commands are listed. |

HP_CALCULATOR

The HP-CALCULATOR command is the QBA simple interactive calculator using reverse Polish notations.

Available OPCODEs (HPC codes) are listed by entering the command HELP.

Use the BACK command to quit and go back to the SYS module.

Input are numbers, + - * / and ^ and OPCODEs. Several numbers and operations can be given on one line. The content of the X register is displayed after each operation.

For example, to compute $2 * \text{EXP}(1.5 * 3 - 30000 / (8 * 1273))$, you should input the following:

```
30000 8/1273/chs 1.5 3 ^ + exp 2 *
```

INFORMATION

Get basic information about topics related to the module you are in.

| Syntax | INFORMATION |
|--------|----------------------------------------------------------------------------------------------------------------|
| | Which subject /Purpose/: <Topic name> |
| Prompt | Specify a subject (or its abbreviation as long as it is unique). Enter a question mark ? for a list of topics. |

MACRO_FILE_OPEN



Some of the information in this topic is related to the add-on Diffusion Module (DICTRA).

The macro file functionality is a way to predefine sequences of Thermo-Calc commands stored in a macro file (a basic text file usually with the default extension *.TCM or *.DCM for DICTRA) and then executing all of the sequences using this command (preceded by the macro file name). This command can be used within various modules (i.e. SYS, POLY, PARROT, TAB and DICTRA_Monitor).

| Syntax | MACRO_FILE_OPEN |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <Name of a macro file *.tcm> |
| | An Open window displays to specify the filename of the macro file (*.TCM) with the macro command, so that the path (in the Look in field) and File name can be specified. |
| | The Files of type *.TCM for Thermo-Calc (Console Mode) calculations and *.DCM for DICTRA simulations, cannot be changed. Click Open or Cancel to continue. |
| | A window such as Save , Open , or Print opens if the macro file contains commands to: |

| Syntax | MACRO_FILE_OPEN |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <ul style="list-style-type: none"> • set log files (these have a file extension .TCM) • save or read GIBBS, POLY or PARROT workspaces • switch user databases • compile experiments (from existing *.POP files) • create new *.PAR files • append *.EXP files • plot diagrams, etc. <p>If required, opening these windows can be avoided by issuing the file names (preferably with file-type extensions; if the files are not in the current working area where the macro is located, the appropriate and complete paths of the files should also be specified) and sometimes with the required options after the corresponding commands or parameters/options.</p> <p>For details, see the related commands and modules.</p> <p>When using a macro file that intended to plot graphs on screen, but the command SET_PLOT_FORMAT is used to alter the plotting environment from the default value, it is important to first use the command SET_PLOT_FORMAT again to change back to the default value.</p> |

This is useful when the same or similar calculations are made frequently with small changes [in terms of system definitions, data manipulations, conditions (for single points, stepping or mapping calculations), plotting settings, etc.). For example, use this feature when calculating phase/property diagrams during an assessment of thermodynamic data.

A macro file can be automatically generated in Console Mode if in the SYS module the SET_LOG_FILE command is used and a log file name (with a file extension *.TCM) is given before any other SYS, DATA, TAB, GIBBS, POLY, POST, PARROT, or ED-EXP command or any special-module command (e.g. BIN, TERN, POTENTIAL, SCHEIL, POURBAIX, or REACTION). Such a log file generated in Console Mode is a text file. You can use a text editor (such as Notepad++) to remove unnecessary command lines, modify some commands, settings and definitions, add some pause points, add comment lines that start with @@, and so forth. Then save it as a macro file with the standard file extension TCM.

Experienced users can also write/edit an appropriate macro file for calculations/simulations, using any basic textual editor outside the Thermo-Calc program.

All commands can be used in a macro file.



The file can be terminated with EXIT or interrupted with SET_INTERACTIVE.

Within a macro file you can use comment-lines (for describing the problems and for explaining commands and inputs/outputs), which should always start with the @@ signs in the beginning of each comment-line. Such comment-lines help to document the macro file, while these are not considered as command lines and thus do not affect the proceeding of all the normal commands in modules when the file is called by Thermo-Calc.

You can put multiple-line comment-blocks in a macro file between the @ (" and "@)" signs. The former sign indicates where the comment begins and the latter sign indicates where the comment ends. A comment-block begins from a line started with the *begin comment* sign @ (and ends with the *finish comment* sign @); all the lines written in between are ignored, and the line started with @) is also ignored.

Another use for a macro file is to allow you to interact at some specific points, using the "@?" sign starting a text line (note that the text describing the expected user-specification/input should be written as a continuous string without any empty space), for user's on-time specifications of arguments/parameters or inputs of parameter-values that are requested by a certain command. The macro temporally stops at the "@?" sign, prompt on screen the text given after "@?", and waits for the specified argument/parameter/value. Thermo-Calc then uses specified argument/parameter/value as the input(s) for the associated command. For example, you can input the values of lower and higher temperature limits for the second axis-variable as follows:

```
GO POLY-3
SET-AXIS-VAR 2 T @?Low-temperature-limit:
@?High-temperature-limit:
```

You can have macro-variables denoted by the signs of @#n (for definition) and ##n (for usage); and up to nine variables inside a single macro file. Such a macro-variable can be assigned with its desired value, as for example:

```
@#3First-element?
```

This writes the text (note that the text describing the expected user specification/input is written as a continuous string without any empty spaces) after the "@#3" sign as prompted on screen and then wait for a specification. The input is assigned to the macro-variable ##3, which is directly called in different parts within the current macro file.

For example, the content of the macro-variable ##3 is inserted in the command:

```
DEFINE-SYSTEM ##3
```

It is also useful in more complicated commands, such as:

```
SET AXIS VAR 1 x(##3) 0 1,,,
```

This command sets the mole fraction of macro variable 3 as axis 1.

A macro file can have any number of pauses at the @& signs, for the purpose of checking the details/results of executing certain commands when running the macro file. However, you can also prevent the software from temporarily stopping at any pause by typing any character (except for the y character for confirming a Yes answer to a command prompt) after specifying the name of a macro file.

A macro file can have a maximum of five nested levels, i.e. a macro file can call another macro file, and if one sub-level macro is terminated by the command it resumes at the next command in the previous macro. If it is terminated by `end-of-file`, the Thermo-Calc (Console Mode) software stops.

This feature is especially useful for alloy design that requires many (hundreds) of calculations/simulations on similar material system/processes (specified in many different but appropriately-documented macro files that are organized in up to five levels) during a certain period of time (e.g. in an evening), you can run the main macro (on the top level) at a certain time (e.g. before leaving the office) and afterwards (e.g. next morning) you can systematically and efficiently check/compare/analyse the results (saved as graphical files, and/or EXP, TXT, XLS... files).

By adding the SYS command SET_ECHO at the beginning of a macro file (or in the primary macro file on the top level if any sub-level(s) of macro files are used), it is useful to automatically display the complete/detailed meaning of various commands in all the sequential operations in the software, all enforced according to the macro file(s).

OPEN_FILE

A text file is opened for use in other commands where a unit number is necessary. The program automatically assigns a unit number.

| | |
|--------|----------------------------------------------------------------|
| Syntax | OPEN_FILE |
| Prompt | File name: <File name> A legal file name must be specified. |

SET_COMMAND_UNITS

This command is useful for reading inputs already prepared by a textual editor on a file. Such inputs can be a table of values or a large number of parameters. The file must be opened with OPEN_FILE.



The first two lines of an input file are skipped before any input is read.

| | |
|--------|--------------------------------------------|
| Syntax | SET_COMMAND_UNIT |
| Prompt | Input unit number /5/: <Input unit number> |

| Syntax | SET_COMMAND_UNIT |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | Specify the input unit number returned from an OPEN_FILE command. The next command is taken from the file connected to this unit number. The last command on such a file must be EXIT or SET_INTERACTIVE when you are in POLY, POST or SYS module, in order to go back to read input from the keyboard. The default value is the current input unit. |
| | Output unit number /6/: <Output unit name> Specify the output unit number returned from an OPEN_FILE command. |

SET_ECHO



This command is not applicable if macro files are not used.

Add the SET_ECHO command at the beginning of a macro *.TCM file (or to the primary macro file on the top level if any sub-level(s) of macro files are used).

Automatically displays on screen the complete details of various commands in all the sequential operations in the software, that are enforced according to the macro file(s).

SET_GES_VERSION

This command enables switching between the two versions of the Gibbs Energy System (GES) calculation engine. As of Thermo-Calc version 2019b, GES6 is the default. Also see ["About the Gibbs Energy System \(GES\) Module" on page 36](#).



GES6 is a re-write and new implementation of the Gibbs Energy System module of Thermo-Calc and it is the default engine. The previous version, GES5, is still available and will continue to work in the background of the program where necessary. The main purpose of GES6 is to support faster development of new features. However, not all GES5 functionality is implemented in GES6. In such cases (except for optimization, PARROT and the POURBAIX module), GES6 falls back silently and uses functionality from GES5 in the background.

| Syntax | SET_GES_VERSION |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | USE GES VERSION 5 OR 6 /6/: |
| Prompt | The default is version 6. If you change the version to GES5, it is set for the current session of Thermo-Calc only. If you launch a new Console window, the version resets to GES6. |

Syntax

SET_GES_VERSION



To globally set the default from GES6 back to GES5, go to the **Tools → Options → "General" on page 37** tab and click **Version 5** for the *Preferred Gibbs Energy System* setting. This is useful if you are using the PARROT module (optimization) or if you have a custom database that is not compatible with GES6.



Contact Thermo-Calc Software AB at info@thermocalc.com for more information about the changes or if you encounter any issues you think are related to the new version of the calculation engine.

SET_INTERACTIVE

Use the SET_INTERACTIVE command to reset the input and output units to the initial values, i.e. keyboard and screen. Add this as the last command to the macro files.

SET_INTERACTIVE_MODE

Use the SET_INTERACTIVE_MODE command to reset the input and output units to the initial values, i.e. keyboard and screen.



Remember to add this as the last command to your macro files, in order to stop execution of the command file in the POST module. It has no meaning in interactive mode.

SET_LOG_FILE

Use it to save, in a basic text file, everything typed into Thermo-Calc. When having problems executing a command sequence, this command can be used to save the command typed onto a log file with the file extension *.TCM.

This command also makes the system echo the full command for all commands typed. This feature is useful when demonstrating the system since the abbreviated commands are often difficult.

The saved log file can then be edited as a macro file by using a basic text editor. This is useful to run the macro file(s) for similar calculations (the same system but slightly varied temperature-pressure-composition conditions), or run the example macro files.



["Macro Files" on page 24](#)

| | |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | SET_LOG_FILE |
| Prompt | A Save window opens to specify a file name for the *.TCM file, so that the path (in the Save in field) and File name can be specified. If a log file with the same name exists in the current working directory, it is overwritten. The Files of type (i.e. TCM) cannot be changed. Click Save or Cancel as applicable. |

SET_PLOT_ENVIRONMENT

Use this command to set the plot devices to save or print plots to, which varies for by installation type. This is preferably set in the initiation file TC.INI.



This command must be terminated with an empty line or two commas.

| | |
|---------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | SET_PLOT_ENVIRONMENT |
| Prompts | <p>Default plot device number /Default number/: <Device number></p> <p>The number given is unique for each type of graphical device. The default graphical device number should normally be selected. A question mark ? gives you a list of all available graphical devices used.</p> |
| | <p>Pseudo file name: <Pseudo-file name></p> <p>The name given here is a symbol which can be used to refer to a physical graphics device when asked for graphical output file.</p> |
| | <p>Plot device number /1/: <Device number></p> <p>The number that specifies the type of graphical device.</p> |
| | <p>Plot file name: <File name or printer name></p> <p>The name of the graphical device on system level (name of file or printer).</p> <p>EXAMPLE</p> <pre>SET_PLOT_ENVIRONMENT 1 lasp 5 a0tr,,</pre> <p>This example sets the default plot device number to 1, and defines an alias named <code>lasp</code> with plot device 5 and connected to a printer named <code>a0tr</code>.</p> |

SET_TC_OPTIONS

Predefine the default values of three general options for performing all the sequential single-points, stepping and mapping calculations.

| Syntax | SET_TC_OPTIONS |
|---------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Use_global_minimization /Y/:</p> <p>By default it global minimization is used where possible (depending on the conditions setting). A global minimization test is performed when an equilibrium is reached. This costs more computer time but the calculations are more robust. Enter N to prevent global minimization being used to reach the equilibrium.</p> |
| | <p>Global_test_interval /0/: <An integer value></p> <p>The integer number determines how often the global minimization should be used during calculations with STEP_WITH_OPTIONS and MAP. If it is set to 0 (zero), the recommended global test interval is used: i.e. every tenth step and at each phase change during step calculations, and only at node points during map calculations. Any other positive integer number, n, suggests it performs global minimization tests at every nth step during step and map calculations. Of course, the Global Minimization test is always carried out at a phase change or a node point. The software is initially configured with 0 (zero) as the default value, but such a configuration for the default value can be changed by this option.</p> |
| | <p>Automatically_add_initial_equilibria /Y/:</p> <p>When ADD_INITIAL_EQUILIBRIUM is not used before a map calculation, a mesh of INITIAL_EQUILIBRIUM is automatically added before the mapping procedure itself takes place. This mesh is only available when the two independent axis-variables have already been defined by the POLY command.</p> |
| | <p>Set_axis_variable</p> <p>If Y is entered, the POLY module always enforces the automatic procedures for adding initial equilibrium points during mapping. For N, no initial equilibrium points are then added during mapping.</p> |

STOP_ON_ERROR

Useful for batch jobs in order to prevent that an erroneous sequence of commands to the program causes waste of computer activity.

| Syntax | STOP_ON_ERROR |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>Give the preferred argument (ON or OFF) after the STOP command. If the default argument ON is given, the program terminates after an illegal or ambiguous command. It is possible to reset the effect of this command by giving the argument OFF.</p> |

Database (TDB) Module Commands



These commands are related to the DATABASE_RETRIEVAL module, which is also known as the TDB module.

Search the online help for step-by-step instructions to define a system.

In this section:

| | |
|--------------------------------|-----|
| AMEND_SELECTION | 123 |
| APPEND_DATABASE | 123 |
| DATABASE_INFORMATION | 123 |
| DEFINE_ELEMENTS | 124 |
| DEFINE_SPECIES | 124 |
| DEFINE_SYSTEM | 125 |
| GET_DATA | 126 |
| LIST_DATABASE | 126 |
| LIST_SYSTEM | 127 |
| REJECT | 127 |
| RESTORE | 128 |
| SET_AUTO_APPEND_DATABASE | 129 |
| SWITCH_DATABASE | 130 |

AMEND_SELECTION



This command is for the DATABASE_RETRIEVAL (TDB) module.

Use this command after defining the elements, species or the system (with the commands DEFINE_ELEMENTS, DEFINE_SPECIES, or DEFINE_SYSTEM). The prompts allow changes to the predefined system. By answering Y or N, each of the selected elements, species or phases can be accepted or rejected (although this is not the case for the constituents or the entire system).

| | |
|---------|-------------------------------------------------------------------------------------------------------------|
| Syntax | AMEND_SELECTION |
| Prompt | Keep <Name1> No/Quit/Yes/ Keep <Name2> No/Quit/Yes/ |
| Options | Keyword-- Elements/Species/Phases name& Names of the pre-defined or pre-selected elements/species/phases |

APPEND_DATABASE



This command is for the DATABASE_RETRIEVAL (TDB) module.

Appends data to the current set of data already read from another database. The syntax is the same as for the SWITCH_DATABASE command.

This command enters all additional functions and parameters to already existing phases, e.g. atomic mobilities, phase constituents, excess models, G0 and interaction parameters.

This command is most commonly used to read mobility data from stand-alone mobility databases.

This command should be used with some caution if thermodynamic data is appended and the application is run with Gibbs Energy System version 5 (see SET_GES_VERSION in the SYS module). It can change calculated values in an unexpected way. This can happen e.g. if the appended database has the same function name as a function in the data retrieved from a database opened with SWITCH_DATABASE.

| | |
|--------|--------------------------------------------------------------------------------------------|
| Syntax | APPEND_DATABASE |
| Prompt | New database name /XYZ/: The name of either an existing database (e.g. FEDEMO) or USER. |

DATABASE_INFORMATION



This command is for the DATABASE_RETRIEVAL (TDB) module.

Use the DATABASE_INFORMATION command to obtain a short description of the current database. This can include information on covered systems, used models, valid ranges for parameters in temperature and composition, major applications, and so on.

DEFINE_ELEMENTS




This command is for the DATABASE_RETRIEVAL (TDB) module.

Define the system in terms of elements. All possible species that can be formed by the given elements are retrieved from the database. The names of elements must be separated with a space or comma. It is possible to use a wildcard * after a common part of element names so that all the elements, which start with that common part and are available in the currently switched or appending database, are defined in the system. Up to 40 elements can be defined into a single system.



Also see ["Defining a System in Console Mode" on page 8](#) for step-by-step instructions to define a system with this command.

| Syntax | DEFINE_ELEMENTS |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | Element& <Element1, Element2, ...> A list of elements to be defined into the system. |
| |  When appending database(s), this command, or DEFINE_SPECIES or DEFINE_SYSTEM must be repeated with the same or similar elements as defined in the first switched database. |

DEFINE_SPECIES




This command is for the DATABASE_RETRIEVAL (TDB) module.

Define the system in terms of species. Only those species given are retrieved. The different names of species must be separated with a space or comma. It is possible to use a wildcard * after a common part of species names so that all the species, which start with that common part and are available in the currently switched or appending database, are defined in the system. Up to 1000 species can be defined in a single system.



["Defining a System in Console Mode" on page 8](#)

| Syntax | DEFINE_SPECIES |
|--------|--------------------------------------------------------------------------------------|
| Prompt | Species& <Species1, Species2, ...> A list of species to be defined in the system. |

| Syntax | DEFINE_SPECIES |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| |  <p>When appending database(s), this command, DEFINE_ELEMENTS or DEFINE_SYSTEM must be repeated with the same or similar elements as defined in the first switched database.</p> |

DEFINE_SYSTEM



This command is for the DATABASE_RETRIEVAL (TDB) module.

Define the system in terms of either elements (equivalent to DEFINE_ELEMENTS) or species (equivalent to DEFINE_SPECIES). Certain databases have a default value of the keyword (as either ELEMENTS or SPECIES) reflecting what is most appropriate when defining a system.

The different names of elements or species must be separated with a space or comma. It is possible to use a wildcard * after a common part of elements or species names so that all the elements or species, which start with that common part and are available in the currently switched or appending database, are defined in the system.

When appending database(s), this command (or DEFINE_ELEMENTS or DEFINE_SPECIES) must be repeated with the same or similar elements as defined in the first switched database. Different databases might contain different elements and have different species definitions: avoid defining elements/species that are missing in the appending database(s). Otherwise, the program indicates these missing elements/species, and ignores them in subsequent steps. But additional elements/species, and additional phases not available in the first switched database can be defined and retrieved from the appending database(s). Up to 40 elements and 1000 species can be defined in a single system.



Also see ["Defining a System in Console Mode" on page 8](#) for step-by-step instructions to define a system with this command.

| Syntax | DEFINE_SYSTEM |
|---------------------|-------------------------------------------------------------------------------|
| Prompt | Elements: <Element1, Element2, ...>, or Species: <Species1, Species2, ...> |
| Options | Description |
| Species or Elements | Default keyword. |
| Element& | Specify a list of elements for the defining system. |
| Species& | Specify a list of species for the defining system. |

GET_DATA



This command is for the DATABASE_RETRIEVAL (TDB) module.

Enter the defined system's elements, species, phases, and the connected parameters obtained from either the primary switched or additionally appending database(s) to the GIBBS and/or DICTRA workspace. Then use the GET_DATA command to get all information concerning a defined system from the databank.



Only after executing this command can you go to any of the application programs such as GES, POLY or DICTRA and use the retrieved data. When appending database(s), this command must be repeated in order to obtain the additional system definitions, parameters and functions.

LIST_DATABASE



This command is for the DATABASE_RETRIEVAL (TDB) module.

List all elements, species, phases or phase constituents in the database.


| Syntax | LIST_DATABASE |
|-------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Options | Description |
| Keyword | One of the keywords Elements, Species, Phases or Constituent must be used to indicate what to list |
| Elements | All available elements, the reference state, atomic mass, H298-H0 and S298. Some elements have spaces in the column for the reference state. This implies that there are no parameters stored for this element. |
| Species | All available species together with the stoichiometric factors. |
| Phases | All available phases together with the number of sublattices and the number of sites in each sublattice. |
| Constituent | All available phases, the number of sublattices, the number of sites in each sublattice and the species dissolved in each phase. Species in different sublattices are separated with a colon (:). It is important to realize, for example, a phase can consist of Fe, Mo, V, and Cr, and its thermodynamic parameters can come from the binary systems Fe-Mo, Fe-V, Fe-Cr, and Mo-Cr. These data can give a relatively good description of the corners of the Fe-Cr-Mo system, but would most certainly give a bad one for the system Mo-Cr-V, due to the fact that the interaction parameters are, by default, set to zero, which originates from binary systems not included in the database. |

LIST_SYSTEM



This command is for the DATABASE_RETRIEVAL (TDB) module.

List all elements, species, phases or phase constituents in the defined system. It works only after a system is defined.

| Syntax | LIST_SYSTEM |
|---------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Keyword | One of the keywords <code>Elements</code> , <code>Species</code> , <code>Phases</code> or <code>Constituent</code> must be used to indicate what to list.  "LIST_DATABASE" on the previous page |

REJECT



This command is for the DATABASE_RETRIEVAL (TDB) module.

Reject elements, species, phases or phase constituents that can form from the defined elements and species. Phases/species/constituents that are possible to form in the defined system are removed from the list of system phases/species/constituents (shown by the command LIST_SYSTEM). Phases/species/constituents that are not included in the list cannot be entered without first being restored. The different names must be separated with a space or comma. You can use a wildcard * after a common part of names so that all the elements/species/phases/constituents that start with that common part and are available in the currently switched or appending database, are rejected from the defined system.

This command can also reject a defined system, and thus reinitiate the entire DATA module memory and GES workspace.

| Syntax | REJECT |
|----------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt 1 | (Keyword = Elements or Species or Phases) If keyword: <Name1, Name2, ...> |
| Prompt 2 | (if keyword = Constituent) Phase: <Phase name> Sublattice number: <Sublattice number in the phase> Constituent: <Constituent(s) in the sublattice of the phase> |
| Prompt 3 | If keyword = SYSTEM the DATA module is reset to its initial state; GIBBS is reinitiated and data already entered to GES is lost. |
| Options | Description and additional information |
| Keyword | One of the keywords <code>Elements</code> , <code>Species</code> , <code>Phases</code> , <code>Constituent</code> or <code>System</code> must be used to indicate what is rejected. |

| Syntax | REJECT |
|-------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Name& | Names of the pre-defined elements/species/phases/constituents/system |
| Elements | The given elements are rejected. |
| Species | The given species are rejected, making it impossible to form them from the defined elements. |
| Phases | The given phases are rejected, making it impossible to form them from the defined elements or species. |
| Constituent | <p>The given constituent in one phase are rejected. Add the following when prompted:</p> <p>Phase: The name of the phase containing the constituent to be rejected.</p> <p>Sublattice number: The sublattice where the constituent enters (the first sublattice is 1). The question is omitted if there exists only one possible sublattice.</p> <p>Constituent: The name(s) of the constituent(s) to be rejected.</p> |

RESTORE



This command is for the DATABASE_RETRIEVAL (TDB) module.

Restore already explicitly rejected elements, species, phases or constituents; it is the opposite of the command REJECT although it does not restore a completely rejected system.

Phases/species/constituents that are possible to form from the defined elements or species are entered to the list of system phases/species/constituents (shown by the command LIST_SYSTEM). Phases/species/constituents that are not included on the list can now be added to the list. The different names must be separated with a space or comma. It is possible to use a wildcard * after a common part of names so that all the elements/species/phases/constituents, which start with that common part and are available in the currently switched or appending database, are restored in the defined system.

| Syntax | RESTORE |
|---------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt1 | <p>(if keyword = ELEMENTS or SPECIES or PHASES)</p> <p>Keyword: <Name1, Name2, ...></p> |
| Prompt2 | <p>(if keyword = CONSTITUENT)</p> <p>Phase: <Phase name></p> <p>Sublattice number: <Sublattice number in the phase></p> <p>Constituent: <Constituent(s) in the sublattice of the phase></p> |
| Options | Description and Information |
| Keyword | One of the keywords Elements , Species , Phases or Constituent must be used to indicate what is rejected. |

| Syntax | RESTORE |
|-------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Name& | Names of the pre-defined elements, species, phases, and constituents |
| Elements | The given elements are restored. |
| Species | The given species are restored and thus possible to form from the defined elements. |
| Phases | The given phases are restored and thus possible to form from the defined elements or species. |
| Constituent | <p>The given constituent in one phase are restored.</p> <p>Add the following when prompted:</p> <p>Phase: The name of the phase containing the constituent to be restored.</p> <p>Sublattice number: The sublattice where the constituent enters (the first sublattice is 1).</p> <p>Constituent: The name(s) of the constituent(s) to be restored.</p> |

SET_AUTO_APPEND_DATABASE



This command is for the DATABASE_RETRIEVAL (TDB) module.

Enforce an automatic action that appends thermodynamic data from a chosen database regarding the system to the data you already have about the system from the current database (that is, the default database or the database last chosen with SWITCH_DATABASE or APPEND_DATABASE).



This is useful to simultaneously retrieve both thermodynamic and mobility data for a defined system when performing a DICTRA module simulation.

This command should be used before defining a system (with the commands DEFINE_ELEMENTS, DEFINE_SPECIES, or DEFINE_SYSTEM) and retrieving the data with the GET_DATA command from the primary switched database.

| Syntax | SET_AUTO_APPEND_DATABASE |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | Database name /XYZ/: <Additional database name> |
| Option | <p>Additional database name</p> <p>The name of an existing database or a User database that corresponds to the automatically-appending database.</p> |

It works in a way that is similar to the APPEND_DATABASE<DATABASE-NAME> command sequence, but only the phases that are also available in the primary switched database are appended. There is no possibility to manually list, reject and/or restore any phase that is available in the appending database. When retrieving data with GET_DATA afterwards, all the

phases that exist in the appending database but not in the primary switched database are automatically rejected. The prompt is kept as for the primary switched database, `TDB_XYZ:` (where `XYZ` stands for the name of the primary switched database) until the execution of `GET_DATA`.

Therefore, to selectively append more phases from a secondary database to a system that is defined and retrieved from a primary switched database, then `APPEND_DATABASE` and sequential commands (such as `DATABASE_INFORMATION`, `DEFINE_SYSTEM`, `DEFINE_ELEMENT`, `DEFINE_SPECIES`, `LIST_SYSTEM`, `REJECT`, `RESTORE` and `GET_DATA`) should be used instead, before this command.

Although it is impossible to manually list, reject and restore any phase from the appending database, the `DATA` module automatically ignores all the phases that do not exist in both the primary switched database and the appending database, and append the data for the phases (that are also available in the primary switched database) from the appending database, as informed on screen when executing `GET_DATA` afterwards.

SWITCH_DATABASE



This command is for the `DATABASE_RETRIEVAL (TDB)` module.

Switch (or change) from the current database to a new one. It also reinitializes the entire module.

The database can be either a standard database (the ones in `tc_initd.tdb`) or a so-called user database. To open your own (user) database, type `USER` followed by the path to the user `.TDB` file or press <Enter> and select it in the window that opens.

| | |
|--------|--------------------------------------------------------------------------------------------|
| Syntax | <code>SWITCH_DATABASE</code> |
| Prompt | New database name /XYZ/: The name of either an existing database (e.g. FEDEMO) or USER. |

POLY Module Commands

In this section:

| | |
|----------------------------------|-----|
| ADD_INITIAL_EQUILIBRIUM | 133 |
| ADVANCED_OPTIONS | 135 |
| AMEND_STORED_EQUILIBRIA | 151 |
| CHANGE_STATUS | 152 |
| COMPUTE_EQUILIBRIUM | 156 |
| COMPUTE_TRANSITION | 158 |
| CREATE_NEW_EQUILIBRIUM | 159 |
| DEFINE_COMPONENTS | 160 |
| DEFINE_DIAGRAM | 161 |
| DEFINE_MATERIAL | 163 |
| DELETE_INITIAL_EQUILIBRIUM | 166 |
| DELETE_SYMBOL | 167 |
| ENTER_SYMBOL | 167 |
| EVALUATE_FUNCTIONS | 170 |
| LIST_AXIS_VARIABLE | 170 |
| LIST_CONDITIONS | 170 |
| LIST_EQUILIBRIUM | 171 |
| LIST_INITIAL_EQUILIBRIA | 172 |
| LIST_STATUS | 172 |
| LIST_SYMBOLS | 173 |
| LOAD_INITIAL_EQUILIBRIUM | 173 |
| MAP | 173 |
| POST | 175 |
| READ_WORKSPACES | 176 |

| | |
|------------------------------|-----|
| REINITIATE_MODULE | 176 |
| SAVE_WORKSPACES | 176 |
| SELECT_EQUILIBRIUM | 178 |
| SET_ALL_START_VALUES | 178 |
| SET_AXIS_VARIABLE | 180 |
| SET_CONDITION | 181 |
| SET_INPUT_AMOUNTS | 183 |
| SET_NUMERICAL_LIMITS | 184 |
| SET_REFERENCE_STATE | 185 |
| SET_START_CONSTITUTION | 187 |
| SET_START_VALUE | 187 |
| SHOW_VALUE | 188 |
| STEP_WITH_OPTIONS | 188 |
| TABULATE | 201 |

ADD_INITIAL_EQUILIBRIUM



This command is for the POLY module.

Add initial equilibrium points from which a phase diagram is calculated (through the MAP command).

For each initial equilibrium the first stage of the mapping varies the value of the given axis variable condition, changing it in the given direction. When a phase change is found it is saved as a start equilibrium, and if the symbol ">" was used, it continues the search until the end of the axis variable.



If no axis variable conditions differ between initial equilibria then the map results in several overlaid diagrams, in accordance with the selected conditions and the values.

The ADD_INITIAL_EQUILIBRIUM default command implicitly makes the MAP command search for phase changes according to settings set by ADVANCED_OPTIONS STEP_AND_MAP command. Default for STEP_AND_MAP are three initial equilibrium equidistantly along each axis variable, along the edge of the axis variable rectangle.

By default these default start points are used in MAP. If any ADD_INITIAL_EQUILIBRIUM is used these default start points are not used. They are again used if the command ADD default is used together with another ADD_INITIAL_EQUILIBRIUM command.

The ADD command with the default direction scans along the axis variables and generates start points each time the scan procedure crosses a phase boundary. In addition, it generates four start points, scanning cross the middle of each axis, if there is any solubility line that does not reach the axes. At the MAP command, a search for lines in the diagram is made along each direction of the axis variables in the diagram.

In this way, it should guarantee that all possible phase boundary lines in a phase diagram are found. It may take a little longer to execute than using the minimum number of start points, as some lines may be calculated more than once. But the POLY module remembers all node points and subsequently stops calculations along a line when it finds a known node point.

It is also possible to create a sequence of start points from one initial equilibria by appending a > after the direction at the ADD command. For example:

```
Direction /Default/: 2>  
Direction /Default/: -2>
```

This generates one start point for each set of phase change in the positive direction of the axis 2 (or negative direction of the axis 2); this ensures finding all possible phase boundary lines (not just the first one) along such an axis direction.

This is particularly useful when you have a phase diagram with several lines with no intersection. It is thus possible to calculate e.g. an isopleth for a much more limited composition range. It is also useful for calculating CVD diagrams and Pourbaix diagrams.

| Syntax | ADD_INITIAL_EQUILIBRIUM |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <div>Direction /Default/: <Direction code></div> <div>Direction code(s):</div> <ul style="list-style-type: none">• 1 or 2 for positive direction of axis 1 or 2, respectively.• -1 or -2 for negative direction of axis 1 or 2, respectively.• Default for MAP to start looking for phase changes from each corner of the axis variable rectangle. <div>The direction is important when the initial equilibrium point is in a single-phase region or when the diagram is an isopleth (tie-lines not in the plane of calculation). In such cases, the program will search for a line in the diagram (i.e., a line where the amount of a phase is zero) in the given direction.</div> |

Normally, this command is not needed to calculate a property diagram (with the STEP_WITH_OPTIONS → NORMAL command-sequence), as the STEP procedure starts from the current equilibrium state already calculated. In many cases, the ADD_INITIAL_EQUILIBRIUM command is not required for MAP commands either.

In order to calculate a simple property diagram, set the equilibrium conditions and the stepping axis variable, and then give a STEP command. But if a phase diagram has disconnected lines, ADD_INITIAL_EQUILIBRIUM may still be needed to add two or more initial equilibria so that the MAP calculation starts from such initial equilibria at the specified directions to find all phase boundary lines.

This command becomes unnecessary in most cases, as the MAP routines that by default use the Global Minimization Technique handles all the initial equilibrium points in a robust and automatic way. Therefore, you do not need to have a good guess of the starting point and to add any initial equilibrium point prior to the calculations of various types of phase diagrams. However, if preferred, use this command to add any initial equilibrium points in certain directions, the POLY module uses the specified starting point(s) and corresponding user-added initial equilibrium point(s) for a mapping calculation; in such a case, the automatic procedure in the rewritten MAP routines are not enforced while the Global Minimization Technique can still be applied. Similar situations occur when a specific database, in which

there are some definitions of initial-equilibrium adding direction(s) for accessed binary and/or ternary subsystems in its ACCESSED_SYSTEM section, is used in the BINARY or TERNARY module for calculating a binary or ternary phase diagram.

All the initial equilibrium points generated by ADD_INITIAL_EQUILIBRIUM (previously and presently; saved in the current POLY workspace) can be easily listed on screen with LIST_INITIAL_EQUILIBRIA. A certain initial equilibrium point (including its conditions and equilibrium results) can be loaded into the current equilibrium, if needed, with LOAD_INITIAL_EQUILIBRIUM. Any specific or all of the initial equilibrium points can be deleted from current POLY workspace, if desired, with DELETE_INITIAL_EQUILIBRIUM.

ADVANCED_OPTIONS



This command is available with the POLY and ED-EXP modules.

| Syntax | ADVANCED_OPTIONS |
|--------|----------------------------------------|
| Prompt | Which option? /Step_and_Map/: <Option> |

Several options are available after you enter this command at the prompt. The default is STEP_AND_MAP.

POLY:advanced-options

Which option? /STEP_AND_MAP/:?

| | | |
|--------------------------|----------------------|-----------------------|
| EQUILIBRIUM_CALCUL | NEW_COMPOSITION_SET | STABILITY_CHECK |
| GLOBAL_MINIMIZATION | OUTPUT_FILE_FOR_SHOW | STEP_AND_MAP |
| IGNORE_COMPOSI_SET_ORDER | PARAEQUILIBRIUM | T-ZERO TEMPERATURE |
| KEEP_COMP_SET_NUMBERS | PHASE_ADDITION | TOGGLE_ALTERNATE_MODE |
| LIST_PHASE_ADDITION | PRESENT_PHASE | |
| MAJOR_CONSTITUENTS | SHOW_FOR_T= | |

Which option? /STEP_AND_MAP/:

- ["EQUILIBRIUM_CALCUL" on page 137](#)
- ["GLOBAL_MINIMIZATION" on page 139](#)
- ["KEEP_COMP_SET_NUMBERS" on page 140](#)
- ["LIST_PHASE_ADDITION" on page 140](#)
- ["MAJOR_CONSTITUENTS" on page 142](#)
- ["NEW_COMPOSITION_SET" on page 143](#)
- ["OUTPUT_FILE_FOR_SHOW" on page 144](#)
- ["PARAEQUILIBRIUM" on page 144](#)
- ["PHASE_ADDITION" on page 147](#)
- ["PRESENT_PHASE" on page 148](#)

- ["SHOW FOR T=" on page 148](#)
- ["STABILITY_CHECK" on page 149](#)
- ["STEP_AND_MAP" below](#)
- ["TOGGLE_ALTERNATE_MODE" on page 150](#)
- ["T-ZERO_TEMPERATURE" on page 150](#)

STEP_AND_MAP



This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.



["ADVANCED_OPTIONS" on the previous page](#)

STEP_AND_MAP is the default ADVANCED_OPTIONS choice and is used to determine how to perform Global Minimization test and how to handle initial equilibrium points.

Settings for MAP and STEP:

```
Global test interval /0/: <Integer number>
```

Settings for MAP:

```
Automatically add initial equilibria /Y/:
```

```
Number of mesh along an axis /3/: <Integer number>
```

```
Use inside meshing points /N/:
```

```
Global test interval /0/: <Integer number>
```

The integer number determines how often the Global Minimization should be used during STEP_WITH_OPTIONS and MAP calculations. If it is set to 0 (zero), the recommended global test interval is used: i.e. every tenth step and at each phase change during STEP calculations, and only at node points during MAP calculations. Any other positive integer number, n , suggests it performs a Global Minimization test at every n -th step during STEP and MAP calculations. Of course, the Global Minimization test is always carried out at a phase change or a node point. The Thermo-Calc software is installed with 0 (zero) as the default value, but such a configuration for the default value can be changed by using SET_TC_OPTIONS in the SYS module.

```
Automatically add initial equilibria /Y/:
```

When ["ADD_INITIAL_EQUILIBRIUM" on page 133](#) is not used before MAP, a mesh of initial equilibrium points are added before the mapping itself takes place. This mesh is only available when two (2) axes are already defined. The default on start-up may be changed by SET_TC_OPTIONS in the SYS monitor.

```
Number of mesh along an axis /3/: <Integer number>
```

An integer for how many intervals of initial equilibrium points to be added along an edge in the diagram. For example, if set to 2 (two), initial equilibrium points are added at the beginning, center, and end of each axis-variable forming 2 intervals.

Use `inside meshing points /N/`:

If N the INITIAL_EQUILIBRIUM mesh consists of initial equilibrium points added only along the edge/border of the diagram defined by the axis-variables. If Y, the initial equilibrium points added are also added to the inside edge.

EQUILIBRIUM_CALCUL



This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.



["ADVANCED_OPTIONS" on page 135](#)

Use this command to decide how to perform the POLY minimization (i.e. the traditional Gibbs energy minimization). The *Global Minimization Technique* is used by default for various single point equilibrium calculations and for stepping or mapping calculations.

To permanently turn off the Global Minimization Technique (for all sequential calculations throughout the current run), use the GLOBAL_MINIMIZATION command and set the options to use only the local POLY minimization. You can also make other adjustments to control the steps in reaching Gibbs energy minima in an equilibrium state, for example.

When enforcing the Global Minimization Technique in the equilibrium calculations, you can further adjust how to assign grid points and to handle compositional set(s) for solution phases during stepping/mapping. In order to improve convergence, and because the Global Minimization Technique uses the normal POLY optimization routine for some calculations, you can also change how to control the steps in reaching Gibbs energy minima in an equilibrium state.

Settings for the Minimization of an Equilibria

The following prompts show how the POLY optimization does the local POLY minimization to reach the minimum of an equilibrium state.

Force positive definite phase Hessian /Y/:

Choose Y or N to determine how to reach the minimum of an equilibrium state in a normal POLY optimization procedure. This is related to the special quantity, the phase stability function $Q_F(\text{phase})$, for all kinds of phases in an equilibrium state [a phase stability function for a phase is negative when the phase composition is inside a spinodal, and positive everywhere else].

If the composition of a solution phase is inside its spinodal, the enforcement of positive definite eigenvalues of a Hessian matrix (i.e. when `Y` is selected) makes the step be taken towards the minima rather than the local maxima. Furthermore, if an eigenvalue (for a phase) of the Hessian matrix is near `0.0`, the step size is large this sets a lower limit to this eigenvalue, reducing the step-size and improving the convergence.



The POLY command sequence `SHOW_VALUE QF(phase)` shows the size of the lowest eigenvalue of a phase in an equilibrium state.

If you answer:

- `Y` , it helps the local POLY minimization to converge (if there is a problem), especially if `QF(phase)=0` for phases.
- `N` the local POLY minimization routine is applied.

For each phase in a defined system, the molar Gibbs energy of the phase is a function of the temperature-pressure condition and its composition:

$$G_m(X) = G_m(T, P; y_1, y_2, \dots, y_n)$$

Compute a Hessian matrix, which describes the curvature of the Gibbs energy curve of this phase at the defined composition `X`:

$$\partial^2 G_m / \partial y_i \partial y_j$$

Diagonalize this matrix and call the Eigenvalues as `e1, e2, ..., en`. The `QF(phase)` quantity for this phase is the lowest of these eigenvalues divided by the same values for a corresponding ideal phase:

$$QF(ph) = \min(\{e_1, e_2, \dots, e_n\}) / \min(\{se_1, se_2, \dots, se_n\})$$

Here, `se1, se2, ..., sen` are the Eigenvalues for the ideal phase. Therefore, for an ideal phase, the `QF(phase)` should always be `1.0`.

`Control stepsize during minimization /Y/:`

Choose `Y` or `N` to determine whether to introduce a control of step size while reaching the minimum of an equilibrium state in a normal POLY optimization procedure. If you choose `Y` it might help the POLY optimization to converge, especially if some site fractions are less than `1E-4`.

GLOBAL_MINIMIZATION



This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

► ["ADVANCED_OPTIONS" on page 135](#)

Designed to decide how to perform the so-called Global Minimization in the POLY module. By default, the POLY module uses the Global Minimization technique for various single-point equilibrium calculations and for stepping or mapping calculations. You can use this to permanently (for all sequential calculations throughout the current software run) turn off the Global Minimization technique and consequently use only the Ordinary POLY Minimization, and additionally adjust the ways to proceed the normal minimization (mainly in terms of how to control the steps in reaching Gibbs energy minima in an equilibrium state). When enforcing the Global Minimization technique in the equilibrium calculations, you can adjust the manners for assigning grid-points and for handling new possible compositional set(s) for solution phases during stepping/mapping; since the Global Minimization technique also uses the normal POLY optimization routine for some calculations, it is also possible to change the ways on how to control the steps in reach Gibbs energy minima in an equilibrium state, in order to improve convergence.

The following prompts affect how the Global Minimization is done. Settings for global minimization:

```
Use global minimization as much as possible /Y/:  
Use global minimization for test only? /N/:  
Maximum number of gridpoints per phase /2000/: <Integer number>  
Use global minimization as much as possible /Y/:
```

Choose Y or N to decide if using the Global Minimization Technique from start of calculation or not. The default value on start-up may be changed by SET_TC_OPTIONS in the SYS module.

If Y the calculation is done when possible (depending on the condition settings), and a Global Minimization test is always performed when an equilibrium is reached. This costs more computer time but the calculations are more accurate.

If N the calculation is not used to reach the equilibrium state. `Use global minimization for test only?` determines if the Global Minimization test is made against the calculated equilibrium states obtained by the Ordinary POLY Minimization calculation.

```
Use global minimization for test only? /N/:
```

If Y a calculated equilibrium state obtained by the Ordinary POLY Minimization calculation is tested against the Global Minimization Technique after it is reached; and if found it as unstable, there is an error message.

If N the Global Minimization Technique is never tested for or done for all sequential calculations throughout the current TCC run. This implies that Global Minimization Technique is permanently turned off, and that consequently only the Ordinary POLY Minimization routine is used.

Maximum number of gridpoints per phase /2000/: <Integer number>

Specify the maximum number of grid points that are computed for each of the phases in the currently defined system, during the calculations enforced by the global minimization. More grid points give a higher robustness and take more computation time. The total number of computed grid points in all phases is limited to 2E6.

KEEP_COMP_SET_NUMBERS



This is available with the ADVANCED_OPTIONS command in the POLY module.



["ADVANCED_OPTIONS" on page 135](#)



["COMPUTE_EQUILIBRIUM" on page 156](#)

This setting affects the COMPUTE_EQUILIBRIUM command and turns on/off the functionality to keep the composition set numbers from the previous equilibrium calculation. The setting is on by default.

To turn the setting on or off enter the ADVANCED_OPTIONS command in POLY, then enter this option and either press <Enter> to keep the default Y or enter N at the prompt:

Keep composition set numbers /Y/:

If this setting is on, performing the COMPUTE_EQUILIBRIUM command keeps the composition set number for any phases that were also present in the last result from COMPUTE_EQUILIBRIUM.



The composition set numbers are kept when the constitution of a phase in the new equilibrium result is similar to the constitution of one of the composition sets of that phase in the previous result. Making major changes to the conditions between calculations makes it therefore less likely that the composition set numbers are kept. The major constituents, given in the thermodynamic database, are used if no previous result exists.

LIST_PHASE_ADDITION



This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

▶ ["ADVANCED_OPTIONS" on page 135](#)

The values set as additional contributions (given by PHASE_ADDITION) to Gibbs energy Gm (J/mol formula unit) to all the phases (stoichiometric or solution) are listed at the current calculated equilibrium.



LIST_PHASE_ADDITION has no additional prompt.

NEW_COMPOSITION_SET



This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

▶ ["ADVANCED_OPTIONS" on page 135](#)

A solution phase that can exist with two (or more) different compositions simultaneously must have two (or more) composition sets in its phase descriptions. Normally the database creates as many composition sets as is necessary but use this command to add or delete more composition sets. A complex solution phase in a defined multicomponent system can have up to 9 different composition sets for the purpose of appropriately handling its possible miscibility gap(s) under various temperature-pressure-composition conditions.

This option is unnecessary if the Global Minimization Technique is in use, as it can automatically detect all possible miscibility gap(s) for complex solution phases (normal or disordered/ordered phases) and then automatically add required composition sets for such phases in the defined system.

This option can automatically create composition sets also for disordered phase when it is executed for the ordered phase.

If you have your own data file, this option must be used to indicate that a solution phase can have a miscibility gap (or may exhibit some complex phase separations as to more than two composition sets), unless that the possibly-additional composition set(s) for the solution phase must have already been added inside the TDB file (through a TYPE_DEFINITION command to amend composition-set) or been manipulated through the GIBBS module (using the AMEND_PHASE_DESCRIPTION COMPOSITION_SET command-sequence). This option asks for default major constituents for the new sets and it is important that this is set correctly, otherwise the test for miscibility gaps may fail.

The following prompts are to specify the additional composition set(s) to handle possible miscibility gap(s) of a certain solution phase:

```
Phase with miscibility gap: <Name of a phase>
```

Specify the name of the phase with miscibility gap.

New highest composition set number /2/: <#>

The default value is usually one higher than the current value. Each phase has initially one composition set. If a lower value is given, composition sets are deleted. You cannot take away the first composition set.

A message displays to show that you need to specify the composition for the composition set # (2,3,...).

Major constituent(s) for sublattice 1: /XX/: <YY>

The major constituents (YY) in each sublattice can be given. This may simplify giving start values when calculating the equilibrium as phases with miscibility gaps should have different major constituents for each composition set.

This prompt is repeated for each sublattice in the phase, sometimes even for all sublattices in the first composition set if such major constituents have not been specified.

MAJOR_CONSTITUENTS



This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.



["ADVANCED_OPTIONS" on page 135](#)

Use this to set the major constituent(s) of a composition sets in a miscibility gap of a solution phase. Normally, the major constituents are specified when a new composition set is created by the NEW_COMPOSITION_SET option; but for the first composition set, this option may be needed before using NEW_COMPOSITION_SET.

The following prompts are to specify the major constituent(s) on each of the sublattice sites for a composition set of a certain solution phase:

Phase name: <name of a phase>

Specify the name of the solution phase with a new set of major constituents.

Composition set number /1/: <#>

The default value for the composition set number (#) is usually /1/ as the other composition sets are given major constituents when creating them. Each phase has initially one composition set.

Major constituent(s) for sublattice 1: /XX/: <YY>

The major constituents (YY) on each sublattice of a solution phase can be given. This may simplify giving start values when calculating the equilibrium as phases with miscibility gaps should have different major constituents for each composition set.

This question is repeated for each sublattice in the phase.

NEW_COMPOSITION_SET



This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.

▶ ["ADVANCED_OPTIONS" on page 135](#)

A solution phase that can exist with two (or more) different compositions simultaneously must have two (or more) composition sets in its phase descriptions. Normally the database creates as many composition sets as is necessary but use this command to add or delete more composition sets. A complex solution phase in a defined multicomponent system can have up to 9 different composition sets for the purpose of appropriately handling its possible miscibility gap(s) under various temperature-pressure-composition conditions.

This option is unnecessary if the Global Minimization Technique is in use, as it can automatically detect all possible miscibility gap(s) for complex solution phases (normal or disordered/ordered phases) and then automatically add required composition sets for such phases in the defined system.

This option can automatically create composition sets also for disordered phase when it is executed for the ordered phase.

If you have your own data file, this option must be used to indicate that a solution phase can have a miscibility gap (or may exhibit some complex phase separations as to more than two composition sets), unless that the possibly-additional composition set(s) for the solution phase must have already been added inside the TDB file (through a TYPE_DEFINITION command to amend composition-set) or been manipulated through the GIBBS module (using the AMEND_PHASE_DESCRIPTION COMPOSITION_SET command-sequence). This option asks for default major constituents for the new sets and it is important that this is set correctly, otherwise the test for miscibility gaps may fail.

The following prompts are to specify the additional composition set(s) to handle possible miscibility gap(s) of a certain solution phase:

Phase with miscibility gap: <Name of a phase>

Specify the name of the phase with miscibility gap.

New highest composition set number /2/: <#>

The default value is usually one higher than the current value. Each phase has initially one composition set. If a lower value is given, composition sets are deleted. You cannot take away the first composition set.

A message displays to show that you need to specify the composition for the composition set # (2,3,...).

Major constituent(s) for sublattice 1: /XX/: <YY>

The major constituents ($\gamma\gamma$) in each sublattice can be given. This may simplify giving start values when calculating the equilibrium as phases with miscibility gaps should have different major constituents for each composition set.

This prompt is repeated for each sublattice in the phase, sometimes even for all sublattices in the first composition set if such major constituents have not been specified.

OUTPUT_FILE_FOR_SHOW



This is an option that is available with the `ADVANCED_OPTIONS` command with the POLY and ED-EXP modules.

► ["ADVANCED_OPTIONS" on page 135](#)

The name of a text file is asked for and all the results output from the command `SHOW_VALUE` is written to this file.

When you use this command, a window opens with a default name for the file `tc_show.dat`. Choose a location to save the file and click **Open**.

PARAEQUILIBRIUM



This is an option that is available with the `ADVANCED_OPTIONS` command with the POLY and ED-EXP modules.

► ["ADVANCED_OPTIONS" on page 135](#)

This calculates a paraequilibrium between two specific phases in an alloy system with one or more interstitial component(s) as fast diffusion species. Under the paraequilibrium state, two partially-equilibrated phases have the same chemical potential (but different contents) for one or more interstitial components (such as C, N, O, S, etc., as individual or combined)], along varied temperature or along a composition variable (of the matrix or one substitutional component) which has already set as the stepping variable with `SET_AXIS_VARIABLE`.

To ensure a successful point calculation of paraequilibrium state between two specific phases in a defined alloy system, it is important that you first have made a single-point equilibrium calculation with an initial overall composition in the current system before performing this advanced-option calculation; however, it is unnecessary to obtain an equilibrium in which either one or both of the target phases is stable. The initial overall composition must have a reasonable setting for the desired paraequilibrium calculation for the two target phases. This is especially true for cases where there are more than one interstitial components to be considered in the paraequilibrium state, because different interstitial components (for example C and N combined) may have significant different behaviors as partitioning into different structured phases; otherwise, for one chosen

interstitial component the initial overall composition is OK for the paraequilibrium calculation between the specified two phases, but for other chosen interstitial component(s) it might be impossible to calculate the paraequilibrium state.

Note the following:

- Always check if the chosen phases A and B have the exactly same definition of elements and if the chosen interstitial components are all in the vacancy sublattice sites of the two phases; otherwise the program cannot find the paraequilibrium state (as it is impossible to correctly calculate u-fractions).
- Always have a comprehensive understanding of the normal phase diagram for the currently investigated system, so that you make the appropriate choice of the phase pair and starting bulk composition for the system.
- Always set the status of the chosen interstitial components as SPECIAL using the POLY command: `CHANGE_STATUSComponent <interstitial component> = SPECIAL`. By doing this, you get a clear picture of u-fractions of various substitutional and interstitial components, which are different from the overall composition in the system. The SPECIAL status means that specified component(s) are not included in summations for mole or mass fractions. Therefore, all the composition variables plotted from paraequilibrium calculations are u-fraction related quantities.

PARAEQUILIBRIUM SETTINGS

Name of first phase: <Phase A>

Name of second phase: <Phase B>

The names of the two target phases A and B, between which the paraequilibrium state is to be calculated, must be entered subsequently or on the same (first) line at once then separated by an empty space, e.g. `FCC#1 BCC` or `FCC#2 M23C6`.



You need to understand what you are dealing with in terms of calculating a paraequilibrium state between the two specified phases.

Specifically, there are four distinguished cases to understand: (1) both chosen phases must have similar interstitial/vacancy sublattices where the fast-diffusion interstitial component (s) occupy; (2) the choice on the target phase pair must be reasonable for the defined system and specified initial overall composition; (3) both target phases should have phase constitution definitions that cover all the defined substitutional and interstitial components of the current alloy system; or (4) it is impossible to calculate the paraequilibrium state between the target phase pairs with given interstitial component(s) in the currently defined system.

```
Fast diffusing component: /c/: <interstitial component(s)>
```

```
Fast diffusing component: /none/: <interstitial component(s)>
```

The name(s) of the fast-diffusing component(s) (C as the default single component) must be given at the above prompts subsequently or at the same (first) prompt. It is possible to specify more than one interstitial component as fast diffusion species.

Note the following:

Such specified interstitial component(s) must be appropriately defined according to the phase constitution definitions of the two selected phases: these must be located on the interstitial/vacancy sublattices in both chosen phases;

If there is only one fast-diffusing component which is carbon, press the <Enter> key to accept the default input at the first prompt; if the single fast-diffusing component is another element (e.g. N), type its name at the first prompt;

If there are two or more fast-diffusing components (e.g. C and N), type their names at the above prompts subsequently or at the same (first) prompt (separated by an empty space, such as C N);

To finish the input of fast-diffusing elements, accept NONE at a repeated prompt, i.e. by pressing <Enter> key to start the paraequilibrium point calculation;

If NONE or a non-existing component name is typed at the first prompt, it means no back diffusion is to be considered, and the para-equilibrium calculation is thus canceled entirely.

If the paraequilibrium state between the two specified phases is successfully calculated, the messages displays e.g.

```
NP(FCC) = 0.3586 with U-fractions C = 2.71821E-02  N = 4.1548129E-03
NP(BCC) = 0.6414 with U-fractions C = 7.10061E-04  N = 2.3781027E-04
All other compositions the same in both phases
Note: LIST-EQUILIBRIUM is not relevant
```

The first and second lines list the phase amounts expressed in mole-percent [NP(phase)] and the contents of the interstitial components C and N in a specific phase expressed in the so-called u-fractions [u-f(phase,C) and u-f(phase,N)], for the phase A (in this case as FCC) and phase B (in this case as BCC), respectively. The third line states that the compositions of the matrix component and all the remaining compositions (regarding substitutional components) in both the target phase A and target phase B are the same at the current paraequilibrium state, while these are not shown on screen. The last line indicates that after this advanced-option calculation the LIST_EQUILIBRIUM command is irrelevant and does not list the paraequilibrium state for the system at the current condition.

However, if the single-point calculation of the paraequilibrium state between the two specified phases has failed, these messages display:

```
*** Error 4 in ns01ad
*** Numerical error
```

This implies that the chosen target phase pair may be unreasonable for the defined alloy system or for the defined initial overall composition, or one or both phases may have inappropriate phase constitution definitions regarding the specified interstitial component (s). Then, you must either modify the settings of initial overall composition or specify the reasonable target phase pair with an appropriate choice of the fast diffusion interstitials in the defined alloy system.

PHASE_ADDITION



This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.



["ADVANCED_OPTIONS" on page 135](#)

Sometimes it is interesting to add a constant contribution to the Gibbs energy of a phase (stoichiometric or solution). This can be done in the Database Module (DATA) or Gibbs Energy Module (GIBBS), for a stoichiometric phase, or for a pure end-member in a solution phase. However, if the addition is related to the equilibrium state, for example, strain energies or surface energies, interfacial energies or deformation energies, it may be more convenient to have this quantity related to the equilibrium state rather than the thermodynamic data.

Give a value of an addition to the Gibbs energy of a phase. The value should always be constant (implying that the addition is not a function of phase composition or temperature-pressure conditions in the equilibrium state) and always be given in the unit of J/mol formula unit of the phase.

The following prompts are to specify the additional energy term (always being a constant) of a given phase.

```
Phase name: <Name of a phase>
```

Specify the name of the (stoichiometric or solution) phase with the addition.

```
Addition to G per mole formula unit: <xxxxxx>
```

The value (xxxxxx) given is added to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy or whatsoever.



It is not composition-, temperature- or pressure-dependent.

PRESENT_PHASE



This is an option that is available with the `ADVANCED_OPTIONS` command with the POLY and ED-EXP modules.

▶ ["ADVANCED_OPTIONS" on page 135](#)

Specify the name of the present phase as the name of the phase that should be present at all calculated equilibria:

Present phase:

Phase name: <Name of a phase>

SHOW_FOR_T=



This is an option that is available with the `ADVANCED_OPTIONS` command with the POLY and ED-EXP modules.

▶ ["ADVANCED_OPTIONS" on page 135](#)

Display various thermodynamic properties (state variables, derived/partial variables or entered symbols) of the currently calculated (stable/meta-stable) equilibrium state but under a different temperature condition. This is useful for knowing, for example, a volume-related property of a frozen (stable/meta-stable) equilibrium state at a certain temperature, where the equilibrated phase assemblage and all the phase compositions are not adjusted while only the temperature condition is changed.

Use this option carefully. You must have successfully calculated a real equilibrium state under one temperature condition (normally the temperature for the last heat treatment). This can then be used to obtain the value(s) of any specified state variable(s) or derived/partial variable(s) or defined symbol(s) for thermodynamic properties of the entire system, of components, or of phases for the currently-defined system (being in a frozen state) under another temperature (normally at room temperature). No real equilibrium is re-calculated through this option, and thus the phase amounts and compositions in the system are the same as at the last real equilibrium calculation.

SHOW_FOR_T= SETTINGS

Temperature (K) /298.15/: <temperature_in_K>

Specify the new temperature condition (in K) under which the values of some specific state variable(s) or derived/partial variable(s) or defined symbol(s) for various thermodynamic properties of the entire system, of components, or of phases) in the currently-defined system (being in a *frozen* state) is shown on screen.

State Variable or symbol /VM/: <State variable or symbol name(s)>

Specify the name(s) of the desired state variable(s) or derived/partial variable(s) or defined symbol(s) for various thermodynamic properties of the entire system, of components, or of phases) in the currently-defined system. More than one state variable or symbol of interest can be simultaneously specified on the same line. For example, you can choose to show the values of VM or GM (i.e. molar volume or molar Gibbs energy of the entire system), or of VM(*) or HM(*).T (i.e. molar volumes or isobaric heat capacity of all phases), or of ACR(*), DGM(*) and LNACR(*,FCC) [i.e. activities of all system components, driving forces for all phases, and activities (in logarithm) of all system components in the FCC solution phase], under the new temperature condition (being in a frozen state).

STABILITY_CHECK



This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.



["ADVANCED_OPTIONS" on page 135](#)

In some composition ranges of a multicomponent system, it often happens that an unstable solution phase region locates inside a miscibility gap, and the stability limit (the *spinodal curve* or *spinodal*) may be not easy to find. A system inside a spinodal is thermodynamically unstable with respect to compositional fluctuations, and the system may experience the *spinodal decomposition* (i.e. decomposing to a mixture of regions with the two stable compositions, one on each side of the miscibility gap).

This option makes it possible to automatically check internal stability of both stable and unstable phases in all subsequent single-point equilibrium and MAP/STEP calculations. It can find out if any phase is subject to spinodal decomposition during the subsequent calculations. If there is an unstable phase located inside a miscibility gap in a calculation, it gives a warning so that you suspend the unstable phase, or use FORCED automatic start values for phase constituents (i.e. SET_ALL_START_VALUES → FORCE command-sequence), or create other composition sets; you can also ignore the warning message if you know that the unstable phase is not formed in the current calculations.

STABILITY_CHECK SETTINGS

Stability check on? /Y/:

Check also for unstable phases? /Y/:

If the automatic stability-check option is switched on choose to also check the stability for unstable phases. The default is Y and if an unstable phase is found to be located in a miscibility gap during a subsequent single-point equilibrium or MAP/STEP calculation, a warning message informs you to selectively make adjustments in the calculation settings [e.g. suspending the unstable phase, or using FORCED automatic start values for phase constituents by the S_A_S_VF command-sequence, or creating other composition sets, etc.]. By answering N the stability check is enforced only to stable phases in the system.

TOGGLE_ALTERNATE_MODE



This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.



["ADVANCED_OPTIONS" on page 135](#)

Toggle the ALTERNATE mode for experimental equilibrium calculation between DEFAULT, ALWAYS and NEVER, during data-assessments using the PARROT optimization.

Set alternate toggle to DEFAULT, ALWAYS, or NEVER?

Set global toggle to DEFAULT, ALWAYS, or NEVER?

- **DEFAULT:** the experiment points are calculated according to the Alternate Technique depending on the SET_ALTERNATE command.
- **ALWAYS:** the experiment points are always calculated according to the Alternate Technique even if the Alternate Mode is switched off in the PARROT module.
- **NEVER:** the experiment points are calculated as normal equilibria even if you SET_ALTERNATE in the PARROT module.

T-ZERO_TEMPERATURE



This is an option that is available with the ADVANCED_OPTIONS command with the POLY and ED-EXP modules.



["ADVANCED_OPTIONS" on page 135](#)

This calculates the temperature when two specific phases have the same Gibbs energy, i.e. the so-called T0 temperature. You must calculate an equilibrium state at an estimated temperature before performing this advanced-option calculation; however, it is unnecessary to obtain an equilibrium state in which either one or both of the target phases is stable.

The following prompts are shown.

Name of first phase: <Phase A>

Name of second phase: <Phase B>

The names of phases A and B must be given, for which the T0 temperature (where the Gibbs energies are equal) is to be calculated.

If the T0 temperature between the two specified phases is successfully calculated, a message displays, e.g.

```
The T0 temperature is 840.82 K. Note: LIST-EQUILIBRIUM is not relevant
```

The first message shows the calculated T0 temperature between the two specified phases.

The second message indicates that after this option calculation with LIST_EQUILIBRIUM is irrelevant and does not list the equilibrium for the system at the T0-temperature.

AMEND_STORED_EQUILIBRIA



This command is for the POLY module.

This command gives information about the calculated blocks (and phase regions included in blocks) after the STEP or MAP calculation(s). It allows you to list all or part of the calculation results, to suspend all or parts of the calculation results that are redundant or where metastable equilibria are calculated, and to restore all or parts of the calculation results (if having been suspended by another AMEND_STORED_EQUILIBRIA command).

The workspace for storing equilibria may overflow during stepping or mapping, and is then written to a file as blocks. Each block usually contains one or more ranges of equilibrium regions.

Use one these options:

- **L** to list the calculated equilibria (all or a specified block)
- **S** to suspend everything (all blocks and their regions)
- **Q** to suspend each set of equilibria individually (specified blocks and/or regions)
- **R** to restore everything (all blocks and their regions)

| Syntax | AMEND_STORED_EQUILIBRIA |
|---------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <pre>Name: <Name of a defined table></pre> <p>List (L) the calculated equilibria, suspend everything (S) or suspend each set of equilibria individually (Q), or restore everything (R).</p> |
| | <pre>Block /*/: <Block number></pre> <p>Specify a block number in the option L, S, Q or R. Or include all the blocks in the amending option, by accepting the wildcard * (press <Enter>).</p> <p>For L, a block (if a block number is specified) or all the blocks (if the wildcard * is accepted/used),</p> |

| Syntax | AMEND_STORED_EQUILIBRIA |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>with the regions and the equilibrium details, that are calculated during stepping or mapping is listed on screen or in a textual file.</p> <p>For Q, each ranger in a block (if a block number is specified) or in all blocks (if the wildcard * is accepted/used) then choose:</p> |
| | <p>S(uspend) K(eep) /K/: <S or K></p> <p>For S or R, if a block is specified, you are asked what region in the block should be suspended or restored. However, if the wildcard * is accepted/used, you are asked the following:</p> <p>Really suspend all /N/:</p> <p>Really restore all /N/:</p> <p>In both cases the default is N and you are prompted for which block(s) and which region(s) in a certain block to execute the S or R action.</p> <p>Really suspend all /N/:</p> <p>Y suspends everything.</p> <p>Really restore all /N/:</p> <p>Y restores everything.</p> |
| | <p>Range: <Range(s) of region></p> <p>Specify one or more ranges to be suspended (the S option) or restored (the R option). The wildcard * suspends or restores all ranges in the specified block.</p> <p>In order to know the ranges the LIST command must first be used.</p> |
| | <p>S(uspend) K(eep) /K/: <S or K></p> <p>The Query suspend option (Q) asks for each region in a certain block if it should be suspended or kept. Suspended regions are not included on sequentially generated plots.</p> |
| | <p>Output file: /Screen/: <File name></p> <p>This prompt is only for listing (the L option), and after it the command is terminated. The file name must be given here; or accept the default Screen (terminal) by pressing <Enter>. A list of stored equilibria as various blocks (with all their ranges) are shown out on screen or the file.</p> |

CHANGE_STATUS



This command is available with the POLY and ED-EXP modules.

In the POLY module, set the status for components, species and phases in the defined system for all the sequential calculations (single-point, stepping and mapping) in equilibrium or local/partial equilibrium state. Each component, species and phase has a status. The default status is ENTERED.

The most important use is to calculate metastable equilibria and metastable phase diagrams by setting some phases (that would otherwise be stable) to the SUSPENDED or DORMANT phase-status. Another important applications is to calculate paraequilibria by setting some components to the SPECIAL component-status.


For a component and for a species, the status can be one of the following:


- **ENTERED:** the component(s) or species are included in the calculation. This is the default status.
- **SUSPENDED:** the component(s) or species are not considered in the calculation.
- **SPECIAL:** the specified component(s) are not included in summations for mole or mass fractions. It only works for component(s).



Only component(s) can have the status SPECIAL, which implies that these are not included in summations for mole or mass fractions.

For example, for the *u-fractions* or other normalized fractions, when one or more of the components are excluded from the summation, you must specify which component(s) should be excluded from the calculation of mole or mass fraction. This component status is particularly useful when calculating paraequilibrium states. Such component(s) are normally interstitial component, and must have the status SPECIAL. This is assigned by the CHANGE_STATUS command.

| Syntax | CHANGE_STATUS |
|---------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>For phases, species or components? /Phases/: <Keyword></p> <p>Keyword = phase or species or components</p> |
| | <p>Phase name(s): <Name(s) of the phase(s)></p> <p>For phase as the keyword, the names of the phases that have their status changed must be given (all on one line). A comma or space must be used as separator. The status to be assigned to the phases can also be given on the same line if preceded with an equal sign (=).</p> <div>  <p>An asterisk, *, can be used to denote all phases. The special notations *S, i.e. a wildcard * directly followed by an S, sign, means all suspended phases. In the same way, *D means all dormant phases, and *E means all entered phases.</p> </div> |
| | <p>Name(s): <Name(s) of the Species or Component(s)></p> <p>For species or components as the keyword, the names of the species or components that have their status changed must be given (all on one line). A comma or space must be used as separator. Similarly to the case of phase as the keyword, the status to be assigned to the species or components can also be given on the same line if preceded with an equal sign =.</p> |

| Syntax | CHANGE_STATUS |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| |  <p>An asterisk, *, can be used to denote all species or components. The special notations *S, i.e. a wildcard * directly followed by an S, sign, means all suspended species or components. In the same way, *E means all entered species or components.</p> |
| | <p>Status /Entered/: <New status></p> <p>The <code>new</code> status to be assigned must be given.</p> <p>For species, the values <code>ENTERED</code> or <code>SUSPENDED</code> can be used.</p> <p>For components, the status <code>ENTERED</code>, <code>SUSPENDED</code> or <code>SPECIAL</code> can be given. <code>SPECIAL</code> means that this component is excluded from sums for mole fractions and mass fractions, which is useful when calculating the <i>ufractions</i> or other normalized fractions of system components.</p> <p>For phases, the status <code>ENTERED</code>, <code>SUSPENDED</code>, <code>DORMANT</code> or <code>FIXED</code> can be given. <code>DORMANT</code> means the same as suspended but the driving force is calculated. <code>FIXED</code> means that it is a condition that the phase is stable at a certain amount.</p> <p>For example, for the <i>ufractions</i>, when one or more of the components are excluded from the summation, you must specify which component should be excluded from the calculation of the mole fraction. This component must have the status <code>SPECIAL</code>. This is assigned by the <code>CHANGE_STATUS</code> command: <code>Change_Status comp C=special</code>.</p> |
| | <p>Start value, number of mole formula units /0/: <Initial amount></p> <p>For <code>ENTERED</code> phases, an <code>initial amount</code> of the phase can be given. Normally, 0 is given if the phase is not likely to be stable, and 0.5 or 1 or any positive number if the phase could be stable, but such an initial amount is only used as the rough starting estimation in the equilibrium calculations.</p> |
| | <p>Number of mole formula units /0/: <Equilibrium amount></p> <p>For <code>FIXED</code> phases, the <code>equilibrium amount</code> of the phase [always using an initial estimation being the <code>NPF(phase)</code> value which it is the normalized mole number of components (per mole formula unit) of the specific status-fixed phase] must be given. If the equilibrium amount is zero, then the phase is at its stability limit.</p> <p>Note when specifying a FIXED phase status</p> <p>Special attention should be paid when specifying a <code>FIXED</code> phase status in equilibrium calculations (for single points, stepping or mapping calculations), as described below.</p> <p>The phase amount variables, <code>NP(phase)</code>, <code>BP(phase)</code> and <code>VP(phase)</code>, as well as all their M/W/V-suffixed quantities, should not be used as conditions. Instead, use the <code>CHANGE_STATUS</code> command to set a relevant condition, e.g. <code>CHANGE_STATUS phase <phase>=fix <amount></code> where the fixed <code><amount></code> is roughly the same as the F-suffixed quantity <code>NPF(phase)</code>.</p> <p>The <code>NPF(phase)</code> quantity is the normalized mole number of components (per mole formula unit) of the specific phase in the defined system, which unlike other F-suffixed state variables [e.g. <code>GF(phase)</code>, <code>HF(phase)</code> and <code>DGF(phase)</code>] cannot be directly applied in any <code>POLY</code> command, implying</p> |

Syntax

CHANGE_STATUS

that it cannot be directly evaluated or listed/shown. If intended to shown such a normalized phase amount value in an equilibrium state, you should use a properly-entered symbol (function or variable), for example: $NPF_{abc} = NP(abc) / NA$ or $NPF_{abc} = NPM(abc) / NA * N$. N is the total system size (in mole). The NA value is a quantity that is phase-dependent (and sometimes also equilibrium-dependent for ionic solution phases), and is the total atomic number in a mole-formula-unit of the specific phase abc (excluding interstitial component and, of course, vacancy). For example, the SIGMA, FCC, BCC and LIQUID phases (among others) in a defined Fe-Cr-Ni-C-N-O system (retrieved from a specific database) may be modeled by certain models, and their NA values must be evaluated in different ways, as described below:

```
LIQUID (C,Cr,CrO3/2,Fe,FeO,FeO3/2,N,Ni,NiO)1 NA = 1
FCC_A1 (Cr,Fe,Ni)1 (Va,C,N,O)1 NA = 1
BCC_A2 (Cr,Fe,Ni)1 (Va,C,N,O)3 NA = 1
SIGMA (Fe,Ni)8 (Cr)4 (Cr,Fe,Ni)18 NA = 30
```

If in the same Fe-Cr-Ni-C-N-O system the liquid solution phase is modeled by the Two-Sublattice Ionic Liquid Model, i.e.:

```
IONIC_LIQ (Cr+3,Fe+2,Ni+2)p (VA,C,N,O-2,FeO3/2)q,7
```

then the evaluation of its NA value becomes even more complicated:

$$NA = p + q * y_{C2} + q * y_{N2} + q * y_{O2} + q * y_{FeO2} / 2$$

where the stoichiometric coefficients p and q are also dependent upon the real equilibrium state (rather than having fixed values in the system). Similar situations occur for other (solid) phases which are described by a multiple sublattice model with ionic constituents, such as SPINEL and HALITE phases in some databases.

There is no strange thing when using a zero value [i.e. 0] in a FIXED phase-status, since it means the specified phase is stable in equilibrium state but has a zero-amount of mass in the equilibrium calculations; in other words, on a phase diagram, the specific phase is on a zero-fraction line (ZFL), i.e. it starts becoming stable on one side of a corresponding phase-boundary line or unstable on the other side of the same boundary. It is often and efficient to do so when calculating e.g. solidus equilibrium states.

However, when a non-zero value [it must always be positive; e.g. 1 or 0.5 or 0.3 or 1.5] is to be specified in a FIXED phase-status, it is unnecessarily the exactly same stable amount of the specific FIXED-status phase in a calculated equilibrium state any longer; instead, the <equilibrium amount> value is the $NPF(\text{phase})$ value that is only roughly used as the estimated starting-value of the FIXED-status phase in the equilibrium calculations.

Therefore, a FIXED-status for a liquid phase being unity does not necessarily imply that it is a liquidus equilibrium state (where the liquid phase is in equilibrium with some solid phases but the liquid phase takes all the mass in the defined system). A unity value for setting the liquid phase status in calculating liquidus equilibrium state can only be used when the liquid mixture phase is predefined as a single-sublattice solution phase (such as metallic liquid phase in multicomponent alloy systems) and the total system size as one mole (i.e. $N=1$).

When a phase is described by a solution model in which two or more sublattices are considered and these sublattice sites may also have different stoichiometric coefficients [meaning that the mixture phase could have more than one atom in formula [$NA>1$; see some examples above], the

| Syntax | CHANGE_STATUS |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>unity value should not be used when setting the FIXED status for the phase; instead, you should use an appropriate value that ranges from 0 to a NPF(phase) value that equals to or is smaller than 1/NA (if the total system size N=1) or 1/NA*N (if N differs from unity). For this reason, if a multicomponent system bears an IONIC_LIQUID phase that is described by the Two-Sublattice Ionic Liquid Model (or any other multiple-sublattice ionic solution phases), it is difficult to use a proper $NPF(ION_LIQ)$ value in setting its FIXED phase-status, because that should be less than (or equal to) the complex value of</p> $N/[p + q \cdot y_{C2} + q \cdot y_{N2} + q \cdot y_{O22} + q \cdot y_{FeO2 \ 3/2}].$ |

EXAMPLES

For example, to obtain the metallic fraction in a system with carbon as an interstitial component, you can set the component status for carbon as `SPECIAL`:

```
Change_Status comp C=special
```



The `SUSPENDED` status for components and species does not always work as expected.

For a phase, it may have one of these statuses:



- **ENTERED**: the phase(s) are included in the equilibrium calculations and these are stable if that minimizes the total Gibbs energy in the defined system. This is the default status for all phases already retrieved from the chosen database(s). An ENTERED phase-status is always associated with an initially-estimated amount [in mole number; normally, as 0 if the phase is not likely to be stable, and as 0.5 or 1 or any positive number if the phase could be stable] but it is only used as the rough starting value in the equilibrium calculations.
- **SUSPENDED**: the phase(s) are not considered in the equilibrium calculations.
- **DORMANT**: the phase(s) are not considered in the equilibrium calculations but their driving forces for precipitation are calculated.
- **FIXED**: it is an equilibrium condition that the status-fixed phase must be stable, and be in equilibrium at a specified amount [always using an initial estimation being the $NPF(phase)$ value which it is the normalized mole number of components (per mole formula unit) of the specific status-fixed phase]. See more descriptions at the end of this command.

COMPUTE_EQUILIBRIUM



This command is for the POLY module.

The full equilibrium state is calculated for the given set of conditions. The Global Minimization Technique is by default enforced in this command (C_E), while it can be disabled temporarily (for the current single-point equilibrium calculation) if using C_E – or C_E * command-combination, or permanently (for all the sub sequential single-point calculations or stepping/mapping calculations within the current TCC run) if having decisively switched it off by a user (or possibly in some special modules) through changing the minimization option using the ADVANCED_OPTIONS → MINIMIZATION_OPTION command-sequence.

| Syntax | COMPUTE_EQUILIBRIUM |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>The C_E command can be used, in order to enforce the ordinary POLY minimization routines in an equilibrium calculation; this is because of that the ordinary C_E command is now associated with the Global Minimization Technique, and only after the Global Minimization</p> <p>If technique is permanently switched off the C_E command makes no difference from the C_E – command-combination.</p> <p>Only certain types of equilibrium conditions [e.g. T, P, N, N(<component>), X(<component>), B, B (<component>), and w(<component>)] are fully supported in the Global Minimization mode (called <i>Direct Global Minimization</i>); and when other types of equilibrium conditions are used, after the initial POLY, a Global Minimization test and corrections are performed until the lowest minimum is found (called <i>Indirect Global Minimization</i>).</p> <p>If there is any problem with convergence, you may try the C_E * command-combination. The character * enforces the command to use an advanced technique to obtain a complex equilibrium. However, after a successful C_E * calculation, you may repeat the C_E command and can check the status of phases, species or components (with LIST_STATUS → CPS command-sequence) and equilibrium conditions (with LIST_CONDITIONS) and list out the calculation results (with LIST_EQUILIBRIUM), because such actions may tell you how to further modify various settings for your current calculation. This command-combination is not that useful anymore, because the Global Minimization Technique that is always associated with the C_E command is even more powerful and more precise in finding the most-stable equilibrium state in a complex heterogeneous interaction system; therefore, the C_E * command-combination is functional and can be used only after the Global Minimization mode has already been disabled temporarily or permanently.</p> <p>Some phases that are not stable in the current equilibrium state may not have their most favorable composition after this command, and thus their driving forces may not be correct. You can force the program to correctly calculate the driving forces of metastable phases, by giving repeated C_E commands until the number of iterations (that is shown on screen after this command) is reduced to 2.</p> <div>  <p>Also see the POLY command SET_NUMERICAL_LIMITS which can set the approximate driving force for metastable phases option on or off in all the subsequent POLY calculations within the current TCC run.</p> </div> <div>  <p>If an equilibrium state for the defined system is not found, an error message is given.</p> </div> <p>You can try repeating this command a few times, or change some of settings for the numerical</p> |

| Syntax | COMPUTE_EQUILIBRIUM |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | limits, for starting variables and starting values, for starting constitutions of certain phases and for reference states of certain components, or to verify some of the defined conditions. |

COMPUTE_TRANSITION



This command is for the POLY module.

This command is a combination of the CHANGE_STATUS, SET_CONDITION and COMPUTE_EQUILIBRIUM commands. It allows a direct calculation when a new phase may form by varying one of the already-set conditions. It can be used only after at least one equilibrium is calculated successfully; otherwise, you are informed on the necessity of first making an equilibrium calculation to find out the stable phases under the current conditions.

When this command is used, the program calls the command CHANGE_STATUS to temporarily change the phase status of a specified phase as FIXED at the *zero* amount, and at the same time to temporarily release one of the existing equilibrium conditions (which is chosen by you). The program calculates a new equilibrium in which that specific phase is stable but its equilibrium amount in the system is zero. The released condition is then assigned with a calculated value that ensures the calculated equilibrium. After wards, the program automatically changes the phase status of that specific phase back to ENTERED, and resets the temporarily released condition as one of the conditions and assigns it with the value that is calculated to ensure the zero-amount formation of that specific phase.

This command is useful to find melting temperature, boiling temperature, or solubility limits, and generally when you want to set the most optimal conditions for calculating an equilibrium where a specific phase becomes stable. It can also be used when you want to know exactly how far away the defined conditions are from the value that can ensure a zero-amount of a specific phase in the system when other conditions remain the same.

After a successful calculation, you can issue a COMPUTE_EQUILIBRIUM calculation to assure the calculated transitional equilibrium is a really stable one, and can also use LIST_EQUILIBRIUM to see the details of transitional equilibrium state.

| Syntax | COMPUTE_TRANSITION |
|---------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Phase to form: <Phase name></p> <p>A new phase name, e.g. BCC that is expected to form, is specified here. This changes the status of this new phase to be FIXED as 0 amount, and the program shows the information such as:</p> <pre>You must remove one of the these conditions P=100000, T=800, N=1, X(FE)=.5 DEGREE OF FREEDOM 0</pre> <p>If the key word ANY is used when prompted for Phase to form (instead of a specific phase name), it is possible to find out any new phase to be formed, in a given varying direction sign and at an estimated change of the released condition: a negative sign means at a lower value of the</p> |

| Syntax | COMPUTE_TRANSITION |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>released condition any new phase is to be found, and a positive sign at a higher value; an estimated change of the released condition implies where any new phase is expected (but it is only estimated value, so any value within its reasonable scale would be enough). Such calculations can be repeated if required. This feature is useful to find out all possible phase transformations along a certain released condition.</p> |
| | <p>Give the state variable to be removed /T/: <One condition></p> <p>One condition must be removed, in order to calculate the transition equilibrium where the specified (or any) new phase to be formed at a calculated value of this released variable.</p> |
| | <p>Therefore, the message may display (after a successful calculation) if, for example, $X(\text{Fe})$ is entered:</p> <pre>To form BCC the condition is set to X(Fe)=.48605791769</pre> <p>This calculated value is assigned as the parameter of that removed condition, in this case, the $X(\text{Fe})$ variable. If the LIST_CONDITIONS command is typed this message displays:</p> <pre>P=100000, T=800, N=1, X(Fe)=4.86057918E-1 DEGREES OF FREEDOM 0</pre> <p>If the key word ANY (instead of a specific phase) is given as the phase name when it is prompted for Phase to form, the line is prompted for a given varying direction sign and an estimated change of the released condition before the calculation of transition equilibrium:</p> |
| | <p>Estimated change (with sign) /1/: <+/-#></p> <p>A given varying direction sign and an estimated change of the released condition, in this case as $X(\text{Fe})$, must be given here: a negative sign means at a lower value of the released condition any new phase is to be found, and a positive sign at a higher value; an estimated change of the released condition implies where any new phase is expected (but it is only estimated value, so any value within its reasonable scale would be enough). For example, if a combination of -0.02 is input, this message may display (after a successful calculation):</p> <pre>To form BCC_A2#1 the condition is set to X(Fe)=.493708756187</pre> <p>This calculated value is then assigned as the parameter of that removed condition, in this case, the $X(\text{Fe})$ variable. The message is shown if the LIST_CONDITIONS command is typed:</p> <pre>P=100000, T=800, N=1, X(Fe)=4.93708756E-1 DEGREES OF FREEDOM 0</pre> |


CREATE_NEW_EQUILIBRIUM



This command is available with the POLY and ED-EXP modules.

During data-assessments using the ED_EXP module (a submodule of PARROT), you can, in the POLY module, create several equilibria with different sets of conditions and phases (but normally with the same set of components). By default, there is one equilibrium. To keep the set of conditions and phase for this equilibrium, create another one using this command, and

use another set of conditions for that. Two equilibria may be useful to calculate easily the enthalpy difference between two states. In the PARROT module, the experimental information is stored as a sequence of equilibria.

| Syntax | CREATE_NEW_EQUILIBRIUM |
|---------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Equilibrium number /2/: <A new equilibrium number></p> <p>Each equilibrium in the POLY workspace is identified by a unique integer number. Such an equilibrium number can be recalled with SELECT_EQUILIBRIUM.</p> |
| | <p>Initiation code /2/:</p> <p>When an equilibrium is created, you can choose to ENTER all components and phases (initiation code 2), ENTER the components only (initiation code 1) or SUSPEND everything (initiation code 0). No other values are legal.</p> <div>  <p>The entered components and phases can later be changed with CHANGE_STATUS.</p> </div> |

DEFINE_COMPONENTS




This command is available with the POLY and ED-EXP modules.


Change the set of components. By default, the elements are used as components. The set of components can be important because some conditions are set using components, for example, the amounts, activities or chemical potentials.

For example, in the system Fe-Si-O, you can define FEO, FE2O3 and SIO2 as components, thus replacing the default FE, SI and O.



This implies a command REINITIATE_MODULE and it should be given as the first command in the POLY module.

| Syntax | DEFINE_COMPONENTS |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Give all new components / existing components/: <New components></p> <p>The new components must be specified all on one line. These replace the existing component definitions.</p> <div>  <p>The number of components cannot be changed with this command. Use CHANGE_STATUS instead.</p> </div> |
| | <p>To keep some existing components, it is recommended that you also enter these on the line. Otherwise, the added new components may not be defined correctly. This is especially important if some components are built out of several elements.</p> |

| Syntax | DEFINE_COMPONENTS |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------|
| |  The new components do not have to be present as species. |

DEFINE_DIAGRAM

This allows automatic calculation and plotting of a diagram with a single command. It is the same as the DEFINE_MATERIAL command up to when the first equilibrium is calculated. The alloy OPTION feature is also available in this command to specify alloying compositions for a special alloy predefined by the OPTION keyword in a selected database (e.g. the TCNI Ni-based Superalloys Database).

Use this command to calculate all types of phase diagrams after specifying all composition value and an initial temperature (if temperature is used as an axis). However, for binary and ternary diagrams, the special BIN and TERN modules may be preferred.

It then lists all the independent variables for the defined system (i.e. temperature and the components) and asks for a variable as the X-axis. You must also specify a maximum and minimum for the X-axis. The second axis (Y-axis) can be another composition (or the temperature if that is not on the X-axis) from the independent variable list. The program then calculates and plots a *phase diagram*, as there are two independent quantities on the axes.


Alternatively, select a dependent quantity as the Y-axis variable from the second list on screen (e.g. the amount of all phases, composition of a specific phase, or fractions of a component in all phases), and the program calculates and plots how this quantity depends on the condition on the X-axis. This is a *property diagram*.

This command ends up within the POST module monitor. You can refine the calculated phase diagram or property diagram.

Moreover, many more property diagrams with axes other than compositions can also be plotted (after the calculation), using SET_AXIS_VARIABLE in the sequent POST monitor.

| Syntax | DEFINE_DIAGRAM |
|---------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>These prompts are given:</p> <p>Same elements as before /Y/?</p> <p>Mole percent of <Element> /##/: <Value></p> <p>or</p> <p>Mass percent of <Element> /##/: <Value></p> <p>Database /ABCDE/: <Database name></p> <p>Major element or alloy: <Element name></p> <p>Composition in mass (weight) percent? /Y/:</p> |

| Syntax | DEFINE_DIAGRAM |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>1st alloying element: <Element name></p> <p>Mass (weight) percent: <Amount of the above specified element></p> <p>2nd alloying element: <Element name></p> <p>Next alloying element: <Element name></p> <p>Mass (weight) percent: <Amount of the above specified element></p> <p>Temperature (c) /1000/: <Temperature of interest in oc></p> <p>Reject phase(s) /none/: <List of phase(s) to be rejected></p> <p>Restore phase(s) /none/: <List of phase(s) to be restored></p> <p>OK? /Y/: <Y or N></p> <p>Should any phase have a miscibility gap check? /N/:</p> <p>Phase with miscibility gap: <phase name></p> <p>Major constituent(s) for sublattice #: /aa/: <Constituent(s)></p> <p>Phase with miscibility gap: <Phase name></p> <p>The first equilibrium is calculated, as with DEFINE_MATERIAL. Then a list of all independent conditions suitable to be chosen as X/Y-axis variables is given by the program.</p> |
| | <p>Quit? /Y/: <Y or N></p> <p>This question is asked only when the axis variables are already defined, or if DEFINE_DIAGRAM is used. It then offers an opportunity to quit (Y) the calculation or to continue (N) the calculation but by defining other axes.</p> |
| | <p>Give the number of the condition to vary /1/: <A condition index></p> <p>Select one of the independent conditions by giving its index on the condition list as the X-axis variable.</p> |
| | <p>Minimum value /XXX/: <minimum value for X-axis></p> <p>Specify the minimum value of the chosen X-axis variable. A default value is shown automatically by the program; press <Enter> to accept it or input another value.</p> |
| | <p>Maximum value /YYY/: <maximum value for X-axis></p> <p>Specify the maximum value of the chosen X-axis variable. A default value is shown automatically by the program; press <Enter> to accept it or input another value. Then another list with some dependent quantities is given by the program, which can be selected as the Y-axis variable.</p> |
| | <p>Give the number of the quantity on the second axis /#/: <##></p> <p>Select one of the independent conditions or dependent quantities as the Y-axis variable, by giving its corresponding index given on the condition lists.</p> <div>  <p>It must be different from the X-axis variable already selected.</p> </div> <p>If selecting one of dependent quantities (by giving the corresponding number from the second list) as the Y-axis, then a property diagram is to be automatically calculated (through a normal</p> |

| Syntax | DEFINE_DIAGRAM |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>stepping procedure) and generated. For composition of a phase the phase name is asked for further specification subsequently.</p> <p>If selecting any of the other independent variables (conditions) on the first list as the Y-axis, then a phase diagram is automatically calculated (through a mapping procedure) and plotted.</p> |
| | <p>Name of phase: /ABC/: <phase name></p> <p>This is prompted only in case of that the composition of a phase is selected as the Y-axis variable. The phase name for which the composition varied along with X-axis variable should be specified.</p> |
| | <p>Multiple start points? /Y/:</p> <p>By default, the program automatically generates and uses multiple start points for mapping the defined phase diagram.</p> |
| | <p>Save file /Result/: <File name></p> <p>The file name where the calculations are stored (saved as a *.POLY3 file) should be specified; the default file name is RESULT.POLY3.</p> <p> Linux and Mac are case sensitive so ensure you enter .POLY3.</p> |

DEFINE_MATERIAL





This command is for the POLY module.


Read data for a system from a database in the POLY module. It is convenient to use for alloys when there is a major component and the amount of the other elements is known in mass (weight) fraction. The command reads the system from the specified database, sets the composition and temperature (and pressure equal to 1 bar) and calculates the equilibrium state before the prompting for a new command. You can list the results with LIST_EQUILIBRIUM or set a new composition or set axis for a STEP or MAP command.




You cannot append data from different databases in this way. Use this command with data from a USER database.

| Syntax | DEFINE_MATERIAL |
|---------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Same elements as before /Y/?</p> <p>This question is asked only if some data is already read from the database, or if the command DEFINE_MATERIAL or DEFINE_DIAGRAM is used. It then offers a convenient way to change the composition and temperature with one command.</p> <p> This command only works properly in cases where the composition of the material system is already defined as in the mole-percent or mass-percent unit.</p> |

| Syntax | DEFINE_MATERIAL |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>Mole percent of <Element> /##/: <Value></p> <p>or</p> <p>Mass percent of <Element> /##/: <Value></p> <p>If you have decided to use the same materials system (available in the current POLY3 workspace) by accepting the default (Y) to the previous prompt <i>Same elements as before /Y/?</i>, one of the alternative prompts display for each of the components in the defined system, depending on how the composition is defined (either in mole-percent, or in mass-percent).</p> <p>Prompts are repeated until all the defined components are completed. Then, the program prompts to specify the temperature condition.</p> |
| | <p>Database /ABCDE/: <Database name></p> <p>The database with the description for the material must be given, or press <Enter> if using the current database. It is possible to give a USER database.</p> |
| | <p>Major element or alloy: <Element name></p> <p>The material must have a major element, usually the element which is present in the largest amount. The fraction of this element is not set but is the rest.</p> <p>In some databases there are the alloys predefined. An alloy has a default major element and have limits of the amounts of the alloying elements. If you stay within these limits the calculation gives reasonable results.</p> |
| | <p>Composition in mass (weight) percent? /Y/:</p> <p>By default the input is taken as mass percent. Choose N to change to mole percent.</p> <div>  <p>Composition should be given in PERCENT not FRACTION, as it is required for the w and x state variables in the SET_CONDITION command.</p> </div> |
| | <p>1st alloying element: <Element name></p> <p>The first alloying element must be given.</p> <p>All alloying elements are asked for in a sequence. These can be given in any order. You must know if you are present as assessed systems in the database. There is no error or warning messages if data are missing. Check the documentation of the database selected.</p> <p>If an alloy is selected, a list of legal alloying elements and their maximum percent is listed on-line.</p> |
| | <p>Mass (weight) percent: <Amount of the above specified element></p> <p>The amount of the alloying element in mass (weight) percent. Using DEFINE_MATERIAL you cannot use the normal flexibility for conditions, but all must be given in mass percent. However, you can after wards change the conditions using SET_CONDITION.</p> |
| | <p>2nd alloying element: <Element name></p> <p>The second alloying element must be given. If only one, press <Enter>. If an element name is</p> |

| Syntax | DEFINE_MATERIAL |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | given then the program asks for its mass fraction. |
| | <p>Mass (weight) percent: <Amount of the above specified element></p> <p>The amount of the above specified alloying element in mass (weight) percent.</p> |
| | <p>Next alloying element: <Element name></p> <p>Continue giving elements and mass (weight) fractions until all elements specified. When all alloying elements and their compositions (as in the above prompt) are specified, press <Enter> as answer to this question to finish the materials definition.</p> |
| | <p>Temperature (C) /1000/: <Temperature of interest in oC></p> <p>POLY makes the first calculation after retrieving the data for this temperature. By pressing <Enter> to accept the default temperature. The value should be given in Celsius (°C).</p> <p> The pressure is set to 1 bar.</p> |
| | <p>Reject phase(s) /None/: <List of phase(s) to be rejected></p> <p>This is a question generated by the database allowing you to select the phases. Normally, all phases should be included when you press <Enter>. If a phase is to be rejected, the name of the phase must be supplied. Several phase names can be specified in one line. It is possible to reject all phase by giving an asterisk *. If the number of phases to be included is much smaller than the total number of phases, it may be convenient to first reject all phases and then restore those that should be included. The question is repeated until you press <Enter> after rejecting all unwanted phases or an asterisk *.</p> |
| | <p>Restore phase(s) /None/: <List of phase(s) to be restored></p> <p>You can restore phases that are accidentally or deliberately rejected. It may also be possible to restore some hidden phases.</p> <p>If phases are to be restored the name of the phases must be supplied. Several phase names can be specified in one line. It is possible to restore all phase by giving an asterisk *. The question is repeated until you press <Enter> after restoring all desired phases.</p> |
| | <p>OK? /Y/:</p> <p>By default, all phases to be selected from the database have the thermodynamic data retrieved and the references from the chosen database are listed. Enter N if there are any errors or you want to amend the selection then you are returned to the prompt about rejecting phase(s).</p> |
| | <p>Should any phase have a miscibility gap check? /N/:</p> <p>The database usually creates two or more composition sets for phases that can have miscibility gaps. However, for some phases this is not done automatically, for example the miscibility gap in the bcc phase in Fe-Cr is usually ignored. But if it is important to include a Cr-rich bcc phase, specify this here. It costs some computation time and may make the subsequent MAP or STEP more difficult to converge.</p> <p>If you do not want to have any phase with a miscibility gap in the calculation, press <Enter>. Then, DEFINE_MATERIAL starts calculating the equilibrium, and is terminated.</p> |

| Syntax | DEFINE_MATERIAL |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>To set such a phase with miscibility gaps in the calculation, answer Y. Then the software asks questions about the phase names and their constitutions, such as:</p> <p>Phase with miscibility gap: <Phase name></p> <p>You must supply the phase name, which has a miscibility gap under the specified system and conditions.</p> |
| | <p>Major constituent(s) for sublattice #: /AA/: <Constituent(s)></p> <p>The software shows a default constituent in the sublattice # (1, 2, 3, ...), according to the existing phase definition in the chosen database. You can specify one or more major constituents for the sublattice # in the phase.</p> <p>This question is repeated until all sublattices are specified.</p> |
| | <p>Phase with miscibility gap: <Phase name></p> <p>You can supply another phase name with a miscibility gap under the specified system and conditions, and answer the questions concerning the major constituent(s) in associated sublattice (s).</p> <p>By pressing <Enter>, the command starts calculating the equilibrium, and then terminates.</p> |
| | <p> It is also possible to use this command to select an alloy from a specific database (e.g. the TCNI Ni-based superalloys database). Such alloys are predefined by the OPTION keyword inside the database, and have their default major elements and composition limits of their alloy elements.</p> <p>Such alloys available in the selected database (at the prompt Database /ABCDE/ can be listed on the screen if typing a ? mark on the prompt Major element or alloy. When a specific predefined alloy (instead of a major element) is selected, the major element is staked from the alloy definition and shown on the screen (with a message like Alloy found with major element NI).</p> <p>You can only specify alloying elements and the compositions (weight percent or mole percent). Typing a ? at any of the prompts for the alloying element names, e.g. 1st alloying element, 2nd alloying element, lists all the alloying elements and the composition limits in the alloy. If the composition of an alloying element is outside of its limit, there is a message (such as Amount above limit: 30.0000) and a prompt Override limit ? /N/. If you decide to enforce the override by answering Y on this prompt (i.e. accepting the over-limit alloying composition), another warning message (such as Amount of major element below limit: 70.0000) and prompt Override limit ? /N/. Then further decide if enforcing the overriding: if Y then accepting the major element's composition below the limit; if N then using the predefined major element composition limit.</p> |

DELETE_INITIAL_EQUILIBRIUM



This command is for the POLY module.

Delete ONE specific initial equilibrium point or ALL of the initial equilibria. The initial equilibria are used as starting points for all the sub-sequential MAP and STEP calculations.

► ["ADD_INITIAL_EQUILIBRIUM" on page 133.](#)

| | |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | DELETE_INITIAL_EQUILIBRIUM |
| Prompt | Number /All/: <Number of an initial equilibrium> |
| | Specify the number of an initial equilibrium (as a specific numerical value e.g. 3, or ALL) to be deleted from the POLY3 workspaces. It is recommended to use LIST_INITIAL_EQUILIBRIA to figure out the numbers for all the existing initial equilibrium points that have already been added (<i>manually</i> through ADD_INITIAL_EQUILIBRIUM, or <i>automatically</i> by some other POLY commands) and stored in the current POLY3 workspace. By default, ALL the initial equilibrium points are deleted. |

DELETE_SYMBOL



This command is available with the POLY and ED-EXP modules.

Use the DELETE_SYMBOL command to remove symbols i.e. constants, variables, functions or tables.

| | |
|--------|---------------------------------------------------------------------------------------------------------------------|
| Syntax | DELETE_SYMBOL |
| Prompt | Name: <Name of a symbol> Specify the name of the symbol to be deleted. Only one symbol can be deleted each time. |

ENTER_SYMBOL



This command is for the POLY module.



There are also a GES and POST module commands with the same name.

Symbols are a useful feature of the POLY and POST modules to define quantities that are convenient. Symbols can be constants, variables, functions or tables.

Functions or tables (with defined functions as values) can be entered in the POST module after a stepping or mapping calculation, for purposes of plotting such entered functions or tables as axis variables.


Within the POLY module, symbols are normally defined prior to an equilibrium calculation (enforced by a C_E command), stepping calculation (enforced by the command STEP_WITH_OPTIONS) or mapping calculation (enforced by MAP). These can be entered after an equilibrium calculation; however, for defined functions, variable or tables, it requires using EVALUATE_FUNCTIONS before showing the corresponding values in the calculated equilibrium state.


The symbols entered in the POST module are not saved in the currently-loaded POLY3 workspaces. Therefore, if you want to apply such symbols in other similar calculations for the same defined system, you must use the ENTER_SYMBOL command prior to the STEPPING or MAPPING calculation in the POLY module.



See [example 44](#) for an example of using variables and functions.

Symbols are a useful feature modules to define quantities that are convenient. Symbols can be constants, variables, functions or tables.

| Syntax | ENTER_SYMBOL |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Constant, Variable, Function or Table? /Function/: <Keyword></p> <p>The Keyword can be specified as CONSTANT, VARIABLE, FUNCTION or TABLE.</p> <ul style="list-style-type: none"> • CONSTANTS can only be entered once and is a means of using a name for a numeric value. For example, the value of 1 atmosphere in Pascal can be denoted by P0 after the command ENTER_CONSTANT P0=101325. Defined constants can be used as values in condition assignments, for example, SET-COND P=P0. • FUNCTIONS are expressions of state variables or other functions. These expressions are saved, and whenever a function value is requested all functions are evaluated. The reason for this is that they may depend on each other. • VARIABLES are similar to functions because they can also be expressions of state variables. However, contrary to functions, they are only evaluated when they are entered or if they are explicitly named in an EVALUATE_FUNCTIONS command. It is possible to enter a variable with a new expression any time. This expression is evaluated directly and its value stored as the value of the variable. Defined variables can be used as values in the SET-CONDITION command. • TABLES are used for listing results from the STEP or MAP commands. A table consists of a list of any number of state variables, functions or variables. Defined tables can also be used in the post-processor POST. <p> There is a special connection between tables and variables. If a variable is used in a table, it is evaluated for each line of the table in the TABULATE command or when the table is used in a plot.</p> |
| | <p>Name: <Name of the symbol></p> <p>Each symbol has a unique name that must start with a letter and can have maximum 8 characters.</p> <p>Legal characters include letters (either UPPER or lower case), digits and underscore _. Any other special character, such as parentheses (and), plus +, minus -, slash / or \, full stop (.), are illegal for symbol names.</p> <p>You can enter the symbol name and the value or function on the same line, these must be separated with an equal sign =, for example, TC=T-273.15 or T_C=T273.15 which stands for a definition of temperature in Celsius. Otherwise, these questions are asked.</p> |

| Syntax | ENTER_SYMBOL |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| |  <p>For different types of symbol (constant, function, variable or table), the questions have different prompts.</p> |
| | <p>Function: <Definition for a function or variable></p> <p><i>Functions</i> and <i>variables</i> are evaluated from an expression of state variables or other functions, constants or variables. The expression is a FORTRAN-like expression and operators +, -, *, = and ** can be used (** only with integer powers).</p> <p>Unary functions like LOG, LOG10, EXP, SIN, COS and ERF can also be used. An expression can be continued on more than one line. An expression should be terminated by a semicolon (;) or an empty line (by pressing <Enter> at the next prompt).</p> <p>Examples of function expressions:</p> <ul style="list-style-type: none"> • GM(LIQUID): The Gibbs energy of liquid per mole component • H.T/4.184: The heat capacity of the system in calories • ACR(CR)/X(FCC,CR): The activity coefficient for Cr in FCC • T-273.15: The temperature in Celsius <p>&: <Continuation of the definition for the symbol></p> <p>The ampersand & means that you can continue to write the function on the new line if one line is not enough for the function. If you finish the function press <Enter> again.</p> |
| | <p>Value: <Value for a constant></p> <p>A <i>constant</i> can only be assigned a numeric value once.</p> |
| | <p>Value or expression: <Value of expression for a variable></p> <p>A <i>variable</i> can be assigned a numeric value or an expression. An expression is evaluated immediately and discarded. Only the numeric value is kept. This gives a possibility to save a value between calculations with different conditions because all state variables and functions are evaluated for the new conditions.</p> |
| | <p>Variable(s): <Variable(s) in a table></p> <p>A <i>table</i> consists of a list of state variables or functions. One way to obtain results from a STEP command is through a table.</p> <p>Example:</p> <pre>ENTER TABLE K=T,X(LIQ,C),X(LIQ,CR),ACR(C)</pre> <p>Which means that the table called K contains four columns, i.e. the temperature, the mole fractions of C and Cr in the LIQUID phase, and the activity of C.</p> <p>To show the temperature in Celsius in a table, give the command ENTER_FUNCTION TC=T-273; and then use the symbol TC in the table.</p> <p>& <Continuation of the definition for the table></p> <p>The ampersand & means that you can continue to write the table on the new line if one line is not</p> |


| | |
|--------|--------------------------------------------------------------------|
| Syntax | ENTER_SYMBOL |
| | enough for the table. If you finish the table press <Enter> again. |

EVALUATE_FUNCTIONS



This command is available with the POLY and ED-EXP modules.

The value of one or more or all entered functions or variables are evaluated and listed.

| | |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | EVALUATE_FUNCTIONS |
| Prompt | <p>Name(s) : <Name(s) of defined function(s)></p> <p>The names of one or more entered functions or variables must be specified. By typing a wildcard *, all functions and variables are evaluated.</p> <p> Variables are evaluated only if these are explicitly named.</p> |

LIST_AXIS_VARIABLE



This command is for the POLY module.

| | |
|--------|---------------------------------------------------------------------------------------------------------------------|
| Syntax | LIST_AXIS_VARIABLE |
| | Lists all the axis variables for a stepping or mapping calculation that have already been set by SET_AXIS_VARIABLE. |

LIST_CONDITIONS



This command is available with the POLY and ED-EXP modules.

All the conditions that are set by the SET_CONDITION command and the command-sequence CHANGE_STATUS PHASE =FIXED <0 or 1 or alike>, are listed. The current conditions are also listed by the LIST_EQUILIBRIUM command. The degree of freedom in the defined system is also shown.

- If this is zero, you can perform a COMPUTE_EQUILIBRIUM command.
- If it is larger than zero, some more conditions are required, and you must further set additional ones, using SET_CONDITION or CHANGE_STATUS.
- If it is negative, then too many conditions are defined and the unnecessary ones conditions need to be removed using the SET_CONDITION command (with a value of NONE for the to-be-deleted condition) or the CHANGE_STATUS command (i.e.

changing a FIXED status of a phase to another type of phase status, ENTERED or DORMANT or SUSPENDED).

| Syntax | LIST_CONDITIONS |
|---------|--------------------------------------------------------------------------------------------------|
| Example | <pre>P=100000, T=800, N(NI)=1E-1, N=1 FIXED PHASES FCC_A1=1 LIQUID=0 DEGREE OF FREEDO 0</pre> |

LIST_EQUILIBRIUM




This command is available with the POLY and ED-EXP modules.

The result (always in SI units) from the last calculated equilibrium is listed on screen or in a text file.



You can also execute this command if no calculation is made or if the calculation fails. Make sure to interpret the results accordingly.

| Syntax | LIST_EQUILIBRIUM |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Output to screen or file /Screen/: <File name></p> <p>The name of the text file where the list of the calculation results shall be written.</p> |
| | <p>Options /VWCS/: <Option(s)></p> <p>Select the output units and formats by optionally specifying a combination of these letters.</p> <ul style="list-style-type: none">• <i>Fraction order</i>: V means VALUE ORDER; A means ALPHABETICAL ORDER.• <i>Fraction type</i>: W means MASS FRACTION; X means MOLE FRACTION.• <i>Composition</i>: C means only COMPOSITION; N means CONSTITUTION and COMPOSITION.• <i>Phase</i>: S means including only STABLE PHASES; P means including ALL NON-SUSPENDED PHASES. <p>Default options are VWCS. If the output fraction type should be in mole fraction (rather than mass fraction), then give VXCS or type X (implying that in this case the options V, C and S are accepted as the listing manners for fraction order, composition and phase).</p> <p>If accepting all the default options, or if accepting all the altered options that had already changed when using this command previously, you can type <code>L_E,,,</code> or <code>LIST_EQUILIBRIUM ,,,</code></p> <div><p>LIST_EQUILIBRIUM displays ORD (ordered) or DISORD (disordered) (when available). See "CHANGE_LEGEND" on page 354 for details.</p></div> |

LIST_INITIAL_EQUILIBRIA



This command is for the POLY module.

List all the equilibria added with ADD_INITIAL_EQUILIBRIUM.

| Syntax | LIST_INITIAL_EQUILIBRIA |
|--------|--------------------------------------------------------------------------|
| | All the initial equilibria are used for the MAP (and STEP) calculations. |

LIST_STATUS




This command is for the POLY module.



There is also an ED-EXP module command with the same name.

List the status of components, species or phases.

| Syntax | LIST_STATUS |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Specify what to list:</p> <p>Option /CPS/ :<keyword(s)></p> <p>keyword = C or P or S, or any combination</p> <ul style="list-style-type: none">• C: list component status• P: list phase status• S: list species status• CS: list both components and species <p>Default is CPS.</p> |
| | <p>The results depend on the key word specified in the options for CHANGE_STATUS, a table with the current status of phases or species or components, or the combinations, is shown:</p> <ul style="list-style-type: none">• For components, the statuses and reference states are listed.• For species, only the status is listed.• For ENTERED and FIXED phases, the status, driving forces and equilibrium amounts are listed. |
| | <p> The metastable phases are listed in descending order of stability. To avoid long outputs only 10 metastable phases (in ENTERED status) are listed by lines, while all other less stable phases are merged onto one line. For DORMANT phases, their phase names and driving forces are listed. For SUSPENDED phases, only the phase names are listed.</p> |

LIST_SYMBOLS



This command is for the POLY module.



There are also POST and ED-EXP module commands with the same name.

Use this command to list the definitions for all constants, functions, variables and tables. In order to find the value of a function or variable, use SHOW_VALUE or EVALUATE_FUNCTIONS. A table is tabulated with the TABULATE command.

| Syntax | LIST_SYMBOLS |
|--------|----------------------------------------------------------------------------------------------------------------------------------|
| | The defined variables are listed up together with the defined functions, but variable names are followed by a percentage sign %. |

LOAD_INITIAL_EQUILIBRIUM



This command is for the POLY module.

Copies all conditions and calculated results from a specific added initial equilibrium to the current equilibrium. The current conditions and calculation results are lost, and the newly loaded initial equilibrium point gets into the POLY workspace.

| Syntax | LOAD_INITIAL_EQUILIBRIUM |
|--------|-----------------------------------------------------------------------------------------------------------------------------|
| | Number: <Number of an initial equilibrium> |
| Prompt | Specify the number of an initial equilibrium to be loaded as current. The number can be found with LIST_INITIAL_EQUILIBRIA. |

MAP



This command is for the POLY module.

This command starts the mapping procedure for making a calculation of phase diagrams in a defined multicomponent heterogeneous system, from one or more initial equilibria. A phase diagram is usually mapped within a specific space that is constructed by two (or more) defined independent mapping axis-variables.

| Syntax | MAP |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | A phase diagram consists of mapped phase boundary lines/curves; on one side of each such phase-boundary line/curve, the amount of one specific stable phase is zero (i.e. the zero-fraction lines). From a single MAP calculation, many different types of phase diagrams in the defined multicomponent heterogeneous system can be plotted, with some desired properties (that vary |

| | |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | MAP |
| | along the calculated phase-region boundaries) plotted as X/Y-axis variables. All different types of phase diagrams are generated by the mapping calculations through this command. |

Normally, you need to have calculated at least one initial equilibrium point and have also defined at least two independent varying variables (i.e. the controlling conditions in the system) that are set with SET_AXIS_VARIABLE. You can also have three, or four or maximum five independent varying variables that are defined by the SET_AXIS_VARIABLE command).

This lists the current values of each of the independent axis variables for each of the calculated equilibrium points along each of the mapped phase boundaries, and also lists the corresponding information when the set of stable phases changes.

The Global Minimization Technique is by default enforced in this command while it can be disabled if having decisively switched it off (or possibly in some special modules) through changing the minimization option using the ADVANCED_OPTIONS → MINIMIZATION_OPTION command-sequence. You can choose how often to do a Global Minimization test (via the Global Test Interval option) in the ADVANCED_OPTIONS STEP_AND_MAP command-sequence.

During a MAP calculation, the values of mapped axis-variables for presenting each phase boundary (lines/points) of the calculated phase-regions are listed, and the corresponding stable-phase sets are shown up.



You can terminate the mapping of a line by pressing a single <Ctrl-A> (Windows) or <Ctrl-C> (Linux). This can be useful in order to stop a longish calculation without losing what is already calculated.

If there is any convergence problem in finding a stable solution at a certain stage during a calculation procedure enforced by this command, these messages display on screen:

```
Convergence problems, increasing smallest site-fraction from
1.00E-30 to hardware precision 2.00E-14. You can restore using
SET-NUMERICAL-LIMITS
```

This implies that smallest site fraction in the current POLY3 workspace is automatically increased from the default value 1.00E-30 to the hardware-dependent precision (under Linux, as 2.00E-14). For other subsequent POLY-module calculation in the current TC run, you can use SET_NUMERICAL_LIMITS to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

In particular, for phase diagrams with tie-lines in the plane (i.e. most binary systems and ternary isotherms), there is a MAP procedure which checks for the best phase to use as axis variables in order to ensure reasonable increments between the tie-lines. This produces smoother curves and also gives a better stability in finding adjacent phase-regions.

Complex miscibility gaps of various solution phases are automatically detected during a mapping calculation, and two or more composition sets for each of such solution phases are automatically generated as well, through an automatic Global Minimization Test procedure (by specifying a Global Test Interval value and confirming the `Automatically add initial equilibria` in the `ADVANCED_OPTION STEP_AND_MAP` command-sequence). As a particular case, such an automatic Global Minimization Test ensures that you can start calculating from high temperatures in an austenitic steel (metallic FCC_A1 solution phase) where the MC carbides/nitrides/carbonitrides (i.e. the C-/N-rich sides of the FCC_A1 miscibility-gap, often (while not always) being referred to as FCC_A1#2, FCC_A1#3, etc.) are not stable, and during the MAP command the MC carbides/nitrides/carbonitrides may first become metastable with a composition different from the metallic FCC_A1 phase and later also stable. The advanced mapping procedure (enforced by the Global Minimization Technique) inside the Thermo-Calc software (both the Console Mode and Graphical Mode) can efficiently and effectively handle complex miscibility gaps in multicomponent heterogeneous systems.

To get a complete phase diagram, sometimes it may be necessary to have multiple starting equilibrium-points, and/or to have added multiple initial-equilibrium points (through `ADD_INITIAL_EQUILIBRIUM`) inside various phase-region boundaries under certain direction(s).

POST



The POST module (post-processor) is a submodule to the POLY module and has its own set of commands. The TAB, BIN, TERN, POT, SCHEIL and POURBAIX modules use the POST module features as part of the automatic generation of the plots.

► ["POST Module Commands" on page 350](#)

► ["Using the POST Module" on page 101](#)

| Syntax | POST |
|--------|-------------------------------------------------------------|
| | Switches to the POST module, which has its own command set. |


READ_WORKSPACES



This command is used in both the POLY and GES (GIBBS) modules.

▶ ["Workspace Files" on page 26](#)

The POLY3 and GIBBS workspaces and the calculated results from the MAP and STEP commands can be READ from a file where they are saved with SAVE_WORKSPACES. Such a *.POLY3 file is not printable.

| Syntax | READ_WORKSPACES |
|---------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Options | <p> File name is the name of a saved POLY3-file where the POLY3 and GIBBS workspaces shall be read from must be specified. You do not need to type the extension if it is the default *.POLY3, otherwise type the whole POLY-file name.</p> <p>A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.</p> <p>A window opens so that the path (in the Look in field) and File name can be specified. The Files of type (i.e. POLY3) cannot be changed. Click Open to open the POLY3 and GIBBS workspaces from the saved *.POLY3 file.</p> <p>When reading back an original POLY3 workspace that has already been saved as an *.POLY3 file in the current Thermo-Calc (Console Mode) run or had been read from an existing POLY3 file under the current work area, while some additional changes in the settings may be made but do not need to be kept in further steps in the current Thermo-Calc (Console Mode) run or any diagram is plotted in the POST module, you can type <code>READ,,</code> or <code>READ_WORKSPACE ,,</code></p> |

REINITIATE_MODULE



This command is for the POLY module.

This command makes sure that the whole POLY module (and thus the entire POLY workspace) is reinitiated to the state as it was when first entered.

| Syntax | REINITIATE_MODULE |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>All the defined components, defined conditions, changed status, entered symbols, defined independent axis-variables, calculated starting equilibrium-points, added initial equilibrium points, stepped/mapped equilibrium data, and so forth, are removed completely. The saved file name is restored to the default.</p> |

SAVE_WORKSPACES



This command is available for both the POLY and GES (GIBBS) modules.

▶ ["Workspace Files" on page 26](#)

You can save the current status and workspaces, including thermodynamic data, conditions, options and results from a single, stepping or mapping calculation on a *.POLY3 file. The workspaces are saved to a file with this command. This is useful so you have access to the workspace for later use or when you need to terminate the current Console Mode session.

- In the Gibbs (GES) module workspace, all thermochemical data are stored.
- In the POLY module workspace, all the last set of conditions and equilibrium state, changed status, entered symbols, advanced options, defined stepping/mapping variables, added initial equilibria, stepped/mapped results, etc., are stored, so it also contain the GES workspace.
- When you are in a response-driven module such as POTENTIAL or SCHEIL for example, a workspace file is automatically opened. In the workspace file, system definitions, conditions for the calculation, calculation results, and plot settings are saved. The file is saved in the current working directory, and is named after the name of the module that created it. For example, the POTENTIAL module saves a workspace file called `POT.POLY3` ; the POURBAIX module saves a file called `POURBAIX.POLY3` and so forth.



After a `SAVE_WORKSPACES` command, you can always come back to exactly the state you had when you issued the command by giving a `READ_WORKSPACE` command. For example, after saving the POLY and GIBBS workspaces to a file, you can leave the program and at a later time `READ` the file and continue from the saved state.

IMPORTANT INFORMATION ABOUT MAP AND STEP COMMANDS





A `STEP` or `MAP` command automatically saves the workspace with the most recently specified name. Do not use the `SAVE_WORKSPACES` command after a `MAP` or `STEP` command.

The results from the `STEP` or `MAP` commands are destroyed by the `SAVE_WORKSPACE` command. You can append several results obtained by sequential `STEP` or `MAP` calculations

without destroying the previous results, whilst SAVE_WORKSPACE erases them all. Keeping this in mind is important and useful particularly for calculating various isothermal (or isoplethal) sections and plotting them on the same diagram in a single Thermo-Calc run.

To suspend some of the STEP or MAP results, use the AMEND_STORED_EQUILIBRIA command.

| Syntax | SAVE_WORKSPACES |
|---------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Options | <p>A <code>file name</code> must be specified. The default extension of the POLY workspace file is *.POLY3 but you can have any other file extension.</p> <p> Linux and Mac are case sensitive so ensure you enter <code>.POLY3</code>.</p> <p>A Save window displays if a file name is not given after the command, so that the path (in the Save in field) and File name can be specified. The Files of type cannot be changed.</p> <p>If there is already a file with the same file name under the directory a warning message displays. Click OK to overwrite the current POLY or GIBBS workspace onto the existing file. Click Cancel to return to the module. You can use the SAVE command with an unspecified name (i.e. through <code>SAVE , , ,</code> command-sequence) to save the POLY or GIBBS workspace.</p> |
| | <p> When saving a POLY3 workspace under a name that already exists under the current work area, which is saved by default (after running a special module, e.g. BIN, TERN, POT, SCHEIL and POURBAIX) or in an earlier stage of the current Console Mode session or in a previous run (which is READ into the current POLY3 workspace), you can type <code>SAVE , , y</code> or <code>SAVE_WORKSPACE , , y</code>. However, this must also be avoided if some results from previous MAP or STEP calculations shall not be destroyed.</p> |

SELECT_EQUILIBRIUM



This command is available with the POLY and ED-EXP modules.

If you create more than one initial equilibrium (during data-assessments using the PARROT/ED_EXP modules), you can switch between them using this command.


| Syntax | SELECT_EQUILIBRIUM |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Number /Next/: <Choice on equilibrium></p> <p>Options: FIRST, LAST, NEXT, PREVIOUS or PRESENT.</p> <p>Most commands affect only the PRESENT equilibrium. However, the REINITIATE_MODULE and DEFINE_COMPONENTS commands remove all the stored equilibria.</p> |

SET_ALL_START_VALUES



This command is available for the POLY and ED-EXP modules.

Set start values, e.g. if the calculation fails or if you have a miscibility gap or ordering. If temperature and pressure are not conditions, you are asked for values of them. Then for each phase prompt on if it should be stable and on its constitution.

| Syntax | SET_ALL_START_VALUES |
|---------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>T /XXXX/: <Temperature in K></p> <p>If the temperature is not a condition, supply a guess of its final value (in K).</p> |
| | <p>P /100000/: <Pressure in Pa></p> <p>If the pressure is not a condition supply a guess of its final value (in Pa).</p> |
| Prompts | <p>Automatic start values for phase constitutions? /N/: <Y, N or F></p> <ul style="list-style-type: none"> For N, enter an initial amount of each entered phase and the major constituents or site fraction of each constituent. For Y, the program automatically sets the start values for phase constitutions in all possible phases. F is for force. In some cases the calculation fails because impossible conditions are set, e.g. $w(C)=1.5$ ($w(C)$ is mass fraction and must thus be less than unity). The program tries to fulfill this condition by putting maximum amount of carbon in all phases, but can fail anyway. When you detect the error and set $w(C)$ to 0.015, the calculation may still fail because it could start from the previous values. To get back to 'fresh' start values, choose F. |
| | <p>Should <phase> be stable /N/: <Y/1 or N/2></p> <p>A guess if this phase should be stable or not is requested. All entered phases are prompted for this question and next two.</p> <div>  <p>You cannot have more phases stable than you have components, but at least one (which dissolves all constituents) must be set as stable. For backward compatibility, this question can be answered by 1 (for Yes) or 0 (for No).</p> </div> <p>The phase name may have a hash sign # followed by a digit, e.g. BCC_A2#2. For phases with miscibility gaps, there should be two phases with the same name but with different numbers after the hash sign.</p> |
| | <p>Major constituent(s): <Name of major constituent(s) in the phase></p> <p>The constituent with the largest fraction in the phase should be specified. If there are more than one constituent with a large fraction, give them all on the same line. If the default major constituents should be used answer with an asterisk (*). By giving \$ the constitution is not changed. If there should be no major constituent give NONE and or if the major constituent(s) are improperly specified, you are asked for individual fractions in the phase.</p> |
| | <p>Y(<phase>,<constituent>) /.XXXXXXXXX/: <.YYYYY></p> <p>The current value (.XXXXXXXXX) is default. You can accept the default by pressing <Enter> or give a new value (.YYYYY).</p> <p>The phase name or constituent name may have a hash sign # followed by a digit, e.g. Y(BCC_</p> |

| | |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | SET_ALL_START_VALUES |
| | A2#2, FE) , Y (BCC_A2#2, C#2) . For phases with miscibility gaps, there should be two phases with the same name but with different numbers after the hash sign. For phases with sublattices, the constituents in sublattice 2 or higher is also be suffixed with a hash sign # followed by a digit. |

SET_AXIS_VARIABLE

In order to calculate a diagram, set at least one axis variable in a stepping calculation, or at least two axis variables in a mapping calculation. For property diagrams, one axis is enough; for phase diagrams two or more are necessary. Any condition that can be set to calculate an equilibrium can be used as an axis variable (with its lower and upper limits and step length) by using SET_AXIS_VARIABLE, and the POLY program does, after a STEP or MAP command, vary the value of the condition between the limits set on its related axis variable. As an extraordinarily unique and powerful feature of the Thermo-Calc software, up to five independent axis variables can possibly be used in a mapping calculation of a multicomponent heterogeneous system; however, the axis numbers 3, 4 and 5 must have chemical potentials of components (or temperature or pressure) as conditions.

| | |
|---------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | SET_AXIS_VARIABLE |
| | Axis number /#/: <An axis number> Specify a number between 1 and 5. The axis numbers 3, 4 and 5 must have chemical potentials of components (or temperature or pressure) as conditions. |
| Prompts | Condition /None/: <One condition> Here the condition that should be varied along the axis must be given. The condition is specified as in SET_CONDITION, for example $w(C)$ for mass fraction of carbon. By accepting NONE, the axis is removed. |
| | Min value /0/: <Min value> Specify the minimum value of the axis condition. |
| | Max value /1/: <Max value> Specify the maximum value of the axis condition. |
| | Increment /.025/: <Step length> Specify the maximum step length. By default, this is 1/40 of the total axis length. |

You can give SET_AXIS_VARIABLE without having set a condition on the axis variable. Under such circumstances, the relevant condition is automatically created and the value set between the minimum and maximum axis limits; however, as a side effect, the POLY module creates two conditions, $P=1e5$ and $N=1$ (these have not been defined as a condition yet), in case you set an axis variable which is not already a condition.

You can use a logarithmic axis during calculations. This is useful for low fractions like in a gas phase where $1e-7$ to $1e-2$ might be an interesting range. The pressure is also suitable for logarithmic step. You specify the logarithmic axis by giving an asterisk * after the increment value.



The increment in this case is treated as a factor.

For example,

```
S-A-V 1 P 1E5 1E25 5*
```

This makes axis 1 a logarithmic axis where the difference between two calculated values makes a factor 5.



The factor must be larger than 1.0.

In some cases, such as when the `DEFINE_DIAGRAM` command is used or a special advanced module (e.g. `BIN`, `TERN`, `POT`, `SCHEIL` or `POURBAIX`) is called, some axis variables are automatically set by the program, not necessarily by this command.

SET_CONDITION




This command is available with the `POLY` and `ED-EXP` modules.

Specify the equilibrium conditions for the calculation. All kinds of state variables, as well as most of the `M/W/V/F`-suffixed state variables (for normalization) and `R`-suffixed state variables (with respect to chosen reference states), can be used as conditions. In addition to temperature and pressure conditions, a multicomponent system can have mixed types of conditions. You should repeat this command for a multicomponent system until the degree of freedom in the defined system becomes zero. When a `FIXED` phase status is used on a specific phase (use `CHANGE_STATUS`), it is equivalent to one condition (implying that particular phase is stable in the defined system).

| Syntax | SET_CONDITION |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | Each condition must be given explicitly, but can be given on the same line (separated by a comma (,) or an empty space) or on separate lines with each one started with the command. |
| | EXAMPLE |
| | SET_COND T=1273, P=1E5, W(C)=.0015, X(LIQ,CR)=.22, ACR(N)=.2 |
| | or |
| | SET_COND T=1273, P=1E5 |
| | SET_COND W(C)=.0015, X(LIQ,CR)=.22 ACR(N)=.2 |

| Syntax | SET_CONDITION |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>In this example, the temperature is set to 1273 K, the pressure to 1 bar (1E5 Pascal), the mass (weight) fraction of C to 0.0015 and the mole fraction of Cr to 0.22 and the activity of N to 0.2.</p> |
| Prompt | <p>State variable expression: <State variable name or linear expression> or a linear expression of state variables.</p> <p>Some of the state variables that can be used in conditions are:</p> <ul style="list-style-type: none"> • T: temperature in the system (in K) • P: pressure in the system (in Pascal) • N: system size (mole number in moles) • B: system size (mass in grams) • N(<component>): mole number of a component in the system • X(<component>): mole fraction of a component in the system • W(<component>): weight fraction of a component in the system • For the SET_CONDITION command this is ACR(<component>): activity of a component in the system. For the SET-ALTERNATIVE_CONDITION command, this is ACR(<phase>,<component>) (activity of a component in a phase) • For the SET_CONDITION command this is MUR(<component>): chemical potential of a component in the system. For the SET-ALTERNATIVE_CONDITION command, this is MUR(<phase>,<component>) (chemical potential of a component in a phase) • X(<phase>,<component>): mole fraction of a component in a phase • W(<phase>,<component>): weight fraction of a component in a phase • ACR(<species>,<phase>): activity of a species in a solution phase • MUR(<species>,<phase>): chemical potential of a species in a solution phase • H: enthalpy in the system (in J) • HM(<phase>): enthalpy of a phase (in J/mol) <p>There are many state variables that can be used in conditions. For more information, enter an <code>INFO STATE_VARIABLES</code> command. A condition is normally a value of a single state variable with its value.</p> <p>EXAMPLE</p> <pre> T=1273.15 P=1E5 X(C)=.002 W(CR)=0.5 ACR(CR)=0.85 X(FCC,C)=.001 H=-250000 HM(BCC)=-225000 </pre> <p>A condition can also be a value of a linear expression involving more than one state variable. For example,</p> <pre> X(LIQ,S)-X(PYRR,S)=0 </pre> |

| Syntax | SET_CONDITION |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>This means that it is a condition that the mole fraction of <i>s</i> component should be the same in the LIQUID and PYRRHOTITE phases. In practice, that should be the congruent melting point.</p> <p> After the equal sign only a numeric value is allowed in the expression.</p> |
| | <p>Factor: <A factor for the state variable, or a continuation></p> <p>This question means you did not answer the previous question. The program is then expecting a single state variable or a complete state variable expression, or the numeric factor in an expression with only one state variable. In a state variable expression a state variable may be preceded by a constant factor. An example of this is:</p> $2 * \text{MUR}(\text{FE}) + 3 * \text{MUR}(\text{O}) = -35000$ <p>This means that it should be a condition that two times the chemical potential of <i>FE</i> plus three times the chemical potential of <i>O</i> should be -35000 J/mol.</p> |
| | <p>State variable: <A specified state variable, or a continuation></p> <p>This question is prompted if a single state variable name has not given in either the prompt <i>State variable expression</i> or <i>Factor</i>, or a state variable expression is given but the expression is incomplete, for example, <i>T-</i> or <i>2*MUR(FE) +</i>, for which the program is then expecting a continuation of the unfinished expression. You need to specify a state variable or a complete state variable expression, or complete the unfinished state variable expression. If a numeric factor is given before this prompt, only one state variable can be specified; otherwise, the program only takes the first state variable to complete the expression (i.e. the factor times the state variable).</p> |
| | <p>Value /X/: <A numeric value, a constant or a variable></p> <p>The value of the condition. This can be a numeric value, a constant or a variable. A suggestion is given as the default value. The special value <i>NONE</i> means that the condition is removed; for example <i>T=NONE</i> takes away the temperature condition.</p> |

SET_INPUT_AMOUNTS


Specify how a system is made up from mixing of various substances. It is useful with a substance database. In the C-H-O-N system, you can, for example, give:

```
S-I-A N(H2)=10, N(H2O)=25, N(C1O2)=5, N(N2)=100
```

The POLY module automatically converts this into conditions for the current set of components. In the case when the elements are defined as the components, the command above is equivalent to

```
SET-CONDITION N(H)=70, N(O)=35, N(C)=5, N(N)=200
```

| Syntax | SET_INPUT_AMOUNTS |
|---------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Quantity: <N(<specie>) or B(<specie>)></p> <p>You can give the amount also preceded with an equal sign = [e.g. <i>N(H2)=10</i> or <i>B(H2O)=1000</i>], or press <Enter> for the next prompt on the amount of the quantity.</p> |

| Syntax | SET_INPUT_AMOUNTS |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>Amount: <Value of the quantity></p> <p>Specify the numerical value of the quantity.</p> <div>  <p>You can give negative amounts in the SET-INPUT-AMOUNTS command.</p> </div> |

SET_NUMERICAL_LIMITS



This command is available for the POLY, Scheil and ED-EXP modules.


Change the criteria for convergence. This is to speed up a calculation in a complex system.

If there is any convergence problem in finding a stable solution at any stage during a calculation procedure enforced by COMPUTE_EQUILIBRIUM, STEP_WITH_OPTIONS, MAP or ADVANCED_OPTIONS), this message displays:

```
Convergence problems, increasing smallest site-fraction from
1.00E-30 to hardware precision 2.00E-14. You can restore using
SET-NUMERICAL-LIMITS
```

This implies that smallest site fraction in the current POLY workspace is automatically increased from the default value 1.00E-30 to the hardware-dependent precision (under Linux, as 2.00E-14). For other subsequent POLY module calculations, you can use this command to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

| Syntax | SET_NUMERICAL_LIMITS |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Maximum number of iterations /500/:</p> <p>By default, the program tries 500 iterations before it gives up. As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.</p> |
| | <p>Required accuracy /1E-6/:</p> <p>This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.</p> |
| | <p>Smallest fraction /1E-12/:</p> <p>This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions.</p> <p>The default value for the smallest site-fractions is 1E-12 for all phases, except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as 1E-30 (unless you have used the SET_NUMERICAL_LIMITS command to reset an even-</p> |

| | |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | SET_NUMERICAL_LIMITS |
| | lower value (e.g. 1E-45, that is naturally enforced to all the phases in the system). |
| | <p>Approximate driving force calculation for metastable phases /Y/:</p> <p>Normally the POLY module only requires that the set of stable phases is in equilibrium in order to terminate the iterations. By default, the metastable phases are included in all iterations but these may not have reached their most favourable composition and thus their driving forces may be only approximate.</p> <div>  <p>If it is important that these driving forces are correct, choose N to force the calculation to converge for the metastable phases. This may require more iterations, and the STEP and MAP command may also terminate due to bad convergence in a metastable phase.</p> </div> |

SET_REFERENCE_STATE



This command is available for the POLY, ED-EXP and POST modules.

The reference state for a component is important when calculating activities, chemical potentials and enthalpies and is determined by the database being used. For each component the data must be referred to a selected phase, temperature and pressure, i.e. the reference state.





All data in all phases where this component dissolves must use the same reference state. However, different databases can use different reference states for the same element/component. It is important to be careful when combining data obtained from different databases.

By default, activities, chemical potentials and so forth are computed relative to the reference state used by the database. If the reference state in the database is not suitable for your purposes, use this command to set the reference state for a component using `SER`, i.e. the Stable Element Reference (which is usually set as default for a major component in alloys dominated by the component). In such cases, the temperature and pressure for the reference state is not needed.

In order to specify conditions in the specific reference state, you can append an `R` to the state variables. Thus, `AC` is the activity (of a system component or of a species in a phase) with respect to the default reference state, and `ACR` is the activity with respect to the selected reference state; `MU` is the chemical potential of a system component with respect to the default reference state, and `MUR` stands for the chemical potential with respect to the

selected reference state. The $_{AC}$ and $_{ACR}$ variables, for both components in a system and species in a phase, can be specified in natural logarithm, e.g. $LNAC(Fe)$, $LNACR(C)$, $LNAC(O2,GAS)$, $LNACR(O2,GAS)$.

For the POST module, and after calculating with the `STEP_WITH_OPTIONS` or `MAP` commands, the reference state for a component can also be changed to plot various properties of the component in the entire system or in a specific phase. Then you can set the diagram axes as the chemical potential or activity quantities with the $_R$ suffix, i.e. $MUR(comp)$, $MUR(comp,ph)$, $ACR(comp)$, $ACR(comp,ph)$ or the common logarithms [e.g. $LNACR(comp,ph)$].

| Syntax | SET_REFERENCE_STATE |
|---------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Component: <Name of the component></p> <p>The name of the component must be given.</p> |
| | <p>Reference phase: <Name of a phase used as the new reference state></p> <p>Enter the Name of a phase for the system.</p> <div>  <p>For a phase to be usable as a reference for a component, the component needs to have the same composition as an end member of the phase. The reference state is an end member of a phase. The selection of the end member associated with the reference state is only performed once this command is executed.</p> </div> <p>If a component has the same composition as several end members of the chosen reference phase, then the end member that is selected at the specified temperature and pressure will have the lowest Gibbs energy.</p> <p>The following are example using temperature. Pressure is used in the same way:</p> <ul style="list-style-type: none"> • In the Fe-C system, BCC can be a reference state for Fe but not for C since BCC can exist as pure Fe but cannot exist as pure C. • If GAS is chosen as the reference phase of component O at such a high temperature that O1 has the lowest energy, then O1 remains the reference state even at calculations performed at lower temperatures where O2 has a lower energy than O1. • Setting the reference state for component O as gas (one sublattice) with constituents O1, O2 and O3 results in O2 being the reference state if, at the present temperature, pure O2 has the lowest energy of O1, O2 and O3. If the reference state is set above a critical higher temperature, then O1 has the lowest energy and consequently becomes the reference state. |
| | <p>Temperature /*/: <Temperature for the reference state></p> <p>Select the Temperature (in K) for the reference state. The wildcard value * means the current temperature is used at the time of evaluation of the reference energy for the calculation.</p> <div>  <p>The temperature set with this command does not affect the temperature used when evaluating the energy of the reference state during the end member selection process.</p> </div> |
| | <p>Pressure /1E5/: <Pressure for the reference state></p> |

| | |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | SET_REFERENCE_STATE |
| | Select the Pressure (in Pa) for the reference state. The wildcard value * means the current pressure is used for evaluating the reference energy at the time of calculation. |
| | <p>EXAMPLES</p> <pre> S-R-S Fe SER S-R-S Cr FCC * 100000 S-R-S H2O AQUEOUS * 100000 S-R-S ZE REF_ELECTRODE * 100000 </pre> |

SET_START_CONSTITUTION



This command is available with the POLY and ED-EXP modules.

This command is similar to SET_ALL_START_VALUES, but is used for an individual phase that may have a wrong constitution.

| | |
|---------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | SET_START_CONSTITUTION |
| Prompts | <p>Phase name: <Name of a phase, and possible major constituent(s)></p> <p>Specify the name of a phase for which the constitution shall be set.</p> <p>If there is a major constituent of the phase, you must specify this on the same line as the phase name. By giving an*, select the default major constituents. A \$ means keeping the same constitution, and NONE means to give individual site-fractions.</p> |
| | <pre>Y(<Phase>#<Composition_set>,<Constituent>#<Sublattice>) /xxx/: <SF></pre> <p>The site fraction (SF) of the constituent shall be given. The default value xxx is the last calculated one.</p> |

SET_START_VALUE



This command is available with the POLY and ED-EXP modules.



This command is not often required as the automatic start values can be handled for most problems.

Set a start value of an individual variable.

| | |
|---------|--------------------------------------------|
| Syntax | SET_START_VALUE |
| Prompts | State variable: <Name of a state variable> |

| | |
|--------|------------------------------------------------------------------------------|
| Syntax | SET_START_VALUE |
| | The state variable must be given. |
| | Value Specify the value to be assigned the state variable as start value. |

SHOW_VALUE



This command is available for the POLY and ED-EXP modules.

Show the current value of any state variable, function or variable.

| | |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | SHOW_VALUE |
| Prompt | State variable or symbol: <Name(s) of state variable(s) or symbol(s)> A single or several state variables or symbols (entered functions or variables) can be specified. |
| | The wildcard * can be used to denote all phases or all components. You can use the dollar-sign \$ to denote all stable phases. Thus, the command SHOW W(*,*)lists the mass fraction of all phases, whereas SHOW W(\$, *) lists the mass fraction of all stable phases. If you SHOW a function, all functions are evaluated using the current values of the state variables. But if you SHOW a variable, it retains its value from the time it was ENTERED or last EVALUATED. Therefore to save a value from one calculation to another, ENTER it to a variable. This is frequently done in the PARROT module to transfer values between equilibria. |

STEP_WITH_OPTIONS



This command is for the POLY module.

The STEP_WITH_OPTIONS (short name, STEP) command initiates the stepping procedure to make a calculation of property diagrams in a multicomponent heterogeneous system. A property diagram is usually stepped under one defined independent stepping axis-variable, and is often constructed by the defined independent mapping axis-variable against a chosen property (for the system, or for a specific phase, or for a certain species).

In the POLY module, it is possible to compute a series of equilibria with one condition as the stepping axis variable. This is achieved by first calculating a single equilibrium, and then

selecting one of the conditions as the axis variable. The minimum and maximum value and the incremental step along the axis must also be given. By default, the global minimization technique is used .



A property diagram consists of property lines that change (normally) along with the stepping axis-variable. From a single STEP calculation, many different types of property diagrams in the defined multicomponent heterogeneous systems can be plotted. Various types of property diagrams are generated by the stepping calculations.

► ["About Property Diagrams" on page 46](#)

Normally, before the command can be invoked, you need to have already calculated an initial equilibrium point and set one independent variable (i.e. the controlling condition in the system) . This is done using SET_AXIS_VARIABLE. You then list the current values of the axis variable for each calculated equilibrium, as well as the corresponding information when the set of stable phases changes.

By default, the global minimization technique is enabled, You can turn this off by using the command-sequence ADVANCED_OPTIONS → GLOBAL_MINIMIZATION.



You can choose how often to do a global minimization test using the command-sequence ADVANCED_OPTIONS → STEP_AND_MAP → GLOBAL TEST INTERVAL.

| Syntax | STEP_WITH_OPTIONS |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | Option? /Normal/: <A chosen option, N, I, S, O, E, M, T, or P> N = Normal, I = Initial equilibria, S = Separate phases, O = One phase at a time, E = Evaluate, M = Mixed Scheil, T= T0, and P Paraequilibrium |

NORMAL (N)

When you accept the default, Normal (N), it allows a stepping calculation with the chosen independently-varying equilibrium condition (axis-variable). Only the step axis value is changed between each step.

When you repeat the STEP → NORMAL command-sequence, you can make several stepping calculations while still keep all the stepping-calculation results in the current POLY3 workspaces.



The calculation results are saved in the default `RESULT.POLY3` file or you can specify to save it in the `<MyName>.POLY3` file. This is as long as there is no `SAVE_WORKSPACES` command before the second set of command sequences (`STEP → NORMAL`). Repeated stepped results can be restored into the same current `POLY3` workspaces/file.



Linux and Mac are case sensitive so ensure you enter `.POLY3`.

The addition of several steps enables you to generate special types of property diagrams and to calculate and plot special phase boundary lines on phase diagrams, such as:

- The missing part(s) of a specific property [that are calculated under another controlling condition inside the range of the stepping-variable] on the same property diagram.
- Two or more sets of a specific property [that are calculated under different controlling conditions and stepped over the same stepping-variable range] on the same property diagram for the same system.
- Calculate some special phase-boundary lines [especially for some defined secondary phase transformations or alike, e.g. the `BCC_A1 <--> BCC_B2` phase-boundary, or equal-Gm for two specific phases, or equal-fraction or equal-activity for a certain species in two specific phases, that shall be calculated under different controlling-conditions and also be stepped over different stepping variable(s)], and then plot (or impose) them onto a corresponding phase diagram (which can be resulted from several such `STEP → NORMAL` calculations or even from a separate `MAP` calculation) for the same system.

INITIAL_EQUILIBRIA (I)

An initial equilibria is added at each calculated point. This can be useful, for instance, to generate a set of isothermal calculations.

When you choose `I`, an initial equilibrium is stored at each calculated equilibria. It is intended to generate a matrix of calculated initial equilibria, first stepped under a `STEP INITIAL_EQUILIBRIA` command-sequence and then repeated by another `STEP NORMAL` command-sequence (or even continued by a `MAP` command).

For example, you can first use the temperature condition as the stepping axis-variable with this option, which calculates a number of initial equilibrium points and automatically adds each one as an initial equilibria for another `STEP → NORMAL` command-sequence (or even for a `MAP` command). Before the second `STEP` command (i.e. the `STEP → NORMAL` command-sequence), you can chose a compositional condition as the new stepping axis-

variable; then the STEP → NORMAL command-sequence uses those created starting equilibrium points (at different temperatures) and steps in such a new compositional variable. As a result, these two STEP commands together give a matrix of values.

SEPARATE_PHASES (S)

In this way, you can calculate how the Gibbs energy for a number of phases varies for different compositions. This is particularly useful to calculate Gibbs energies for complex phases with miscibility gaps and for an ordered phase that is never disordered (e.g. SIMGMA-phase, G-phase, MU-phase, etc.).

ONE_PHASE_AT_TIME (O)

This option is recommended for STEPPING heterogeneous systems with both ordered phases and the disordered pairs.

When you choose **O**, the stepping calculation is conducted individually for one phase at a time. That is, it is stepped over the whole stepping variable range, but the stepping is repeated for all the entered phases in the defined system. This is particularly useful to properly step in composition for an equilibrium heterogeneous system with both ordered phases and the disordered pairs. Thus, instead of calculating for the same composition for each of the phases at each composition step, it starts the stepping in each of the phases in the default most-stable compositions (the major constitutions).

EVALUATE (E)



For Scheil-Gulliver simulations it is recommended you use the SCHEIL module.

Evaluate **E** is an advanced option and is useful when additional conditions (instead of the stepping variable) require changing during a stepping calculation. It allows a stepping calculation in a single axis with simultaneous evaluation of one or more variables after each step. As variables can be used as conditions, it means that you can change the conditions during the stepping. After a successful EVALUATE calculation, you can go to the POST module to manually define and plot property diagrams.



The variables given are evaluated after each step, which may change other conditions. This can be useful to perform the Ordinary ScheilGulliver Approach (non-equilibrium transformations) for simulating alloy solidification without back diffusion of fast-diffusing interstitial components in solid phases. However, it is recommended you use the SCHEIL module.

Specify the prompt:

Variable name(s): <Variable name>

The names of the variables that shall be evaluated after each step must be typed here.



The miscibility gap test is automatically used during stepping (see ["ADVANCED OPTIONS" on page 135](#)) if a phase has two or more composition sets.

The miscibility gap test means that you can start calculating from high temperatures in a steel where the MC carbide is not stable. During the calculation, the MC carbide first becomes metastable with a composition different from the metallic FCC phase and later also becomes stable.



See Console Mode example tcex30A.

MIXED_SCHEIL (M)



For Scheil-Gulliver simulations it is recommended you use the SCHEIL module.

This is an advanced stepping calculation designed for the Extended Scheil-Gulliver Approach (partial-equilibrium transformations) to simulate alloy solidifications with back diffusion of one or more fast-diffusing interstitial components (such as C, N, O, S, etc.) in solid phases is performed. It also will consider BCC-->FCC phase transformation (practically for steels) along the alloy solidification process.

To ensure a successful stepping calculation of mixed Scheil-Gulliver simulation of solidification process of a defined alloy system with a certain initial overall composition, it is important to note the following:

- For solution phases with possibility of miscibility gap existence, you have appropriately added the necessary composition set(s);

- You have already set the temperature condition as the stepping SET_AXIS_VARIABLE command, with minimum and maximum temperature points as well as an appropriate s temperature step for the cooling process).
- There must be a composition condition for each of the back diffusion components (i.e. fast-diffusing interstitial components, such as C, N and/or other elements) that are already defined in terms of mole-fraction or mass-fraction, e.g. $x(C)$ and $w(N)$. Otherwise, a stepping calculation with this option can fail.
- An initial equilibrium in which the LIQUID mixture phase is the only stable must be calculated. This is why it is good to start with a relatively high temperature condition for the initial equilibrium calculation. It is always necessary to reject or suspend the GAS mixture phase (if it exists) before the C-E and STEP commands, to avoid its formation along with LIQUID.
- In cases where fast-diffusing interstitial components are specified as back diffusion components, you can choose to `allow BCC>FCC` phase transformation (practically for steels) during the alloy solidification process.

These are the prompts for this option:

Fast diffusing components: <Fast diffusion interstitial(s)>

Specify one or more interstitial component(s) as the back diffusion component(s).

- If there is only one fast-diffusing interstitial component (e.g. C or N), type its name;
- If there are two or more fast-diffusing interstitial components (e.g. C, N and S), always type the names on the same line at once (separated by an empty space in between, e.g. C N S);
- If there is no fast-diffusing interstitial component to be considered, type `NONE` to ignore back diffusion entirely, meaning a normal Scheil-Gulliver simulation is performed.



Such specified back diffusion interstitial component(s) must be appropriately defined according to the phase constitution definitions of some major alloy solution phases (e.g. FCC, BCC, HCP, etc.). These are located on the interstitial/vacancy sublattices in such alloy solution phases; otherwise, such a Scheil-Gulliver simulation may not make sense at all.

Allow BCC -> FCC ? /Y/:

By default the BCC-->FCC phase transformation is allowed. This is usually a typical phenomenon along the cooling processes of steels/Fe-alloys.

During the calculation the simulated solidification path, including the locally-equilibrated phase assemblage (region), captured temperature condition (T in K), remaining liquid phase (N_L , mole fraction), overall formed solid phases (N_S , mole fraction) and latent heat formation (N_H , J/mol) along the cooling process are shown after the information on starting temperature point of the alloy solidification process, e.g.

```
Solidification starts at 1743.15 K
Phase Region from 1.744150E+03 for: LIQUID
Phase Region from 1.742525E+03 for:
    LIQUID
    FCC_A1#1
    1742.5250      0.9960      0.0040      -1.1824
    1742.4000      0.9795      0.0205      -202.1585      . . . . .
Phase Region from 1.733150E+03 for:
    LIQUID
    BCC_A2
    FCC_A1#1
    1733.1500      0.3294      0.6707      -8032.6240
    1733.0250      0.3237      0.6763      -8095.1490      . . . . .
```

After a successful calculation, you can go to the POST module to manually define and plot property diagrams for the alloy solidification process according to the chosen Scheil-Gulliver model, or to impose existing relevant experimental information or other types of calculated solidification results [e.g. Scheil-Gulliver simulation with or without considering fast-diffusing interstitial component(s), full-equilibrium approach, or Diffusion Module (DICTRA)-type simulation with moving-boundary conditions] onto the same plotted property diagrams. Normally, the solidus temperature (T in Celsius) is set as one of the axis variables (usually as Y-axis in most cases), while the other plotted quantity on the other axis can be the amount of overall formed solid alloy phases (N_S in mole-fraction or B_S in mass-fraction), the amount of remaining liquid phase (N_L in mole-fraction or B_L in mass fraction), the heat of latent along the solidification process (N_H in J/mol or B_H in J/gram), among many other properties in the solidified alloy phases or in the whole alloy system.

T-ZERO (T)



See Console Mode example 41.

This advanced option allows a stepping calculation of the so-called T0 (T-zero) line in a diffusionless transformation (where two specific partially-equilibrated phases have the same Gibbs energy) along a composition variable which has already set as the stepping variable with ["SET_AXIS_VARIABLE" on page 180](#).



The temperature condition cannot be set as the stepping variable if you want to make a STEP T-ZERO calculation.



Prior to performing the step T0 command sequence, and to ensure a successful calculation of T0 line between two specific phases after an initial equilibrium calculation in the current system, it is sometimes recommended to make a single T0 point calculation using ADVANCED_OPTIONS → T-ZERO.

Specify these prompts:

Name of first phase: <Phase A>

Name of second phase: <Phase B>

The names of the target phases, for which the Gibbs energies equal to each other at each point on the T0 line, must be entered.

During the calculation, the T0 values are shown after the corresponding scanned conditions (of the stepping composition variable), e.g.

```
Phase Region from 1.000000E-01 for:
```

```
  BCC_A2
  FCC_A1
1.000000E-01      940.24
9.250000E-02      941.20
. . . . .
2.500000E-03      977.61
7.500000E-09      979.34
```

```
Phase Region from 1.000000E-01 for:
```

```
  BCC_A2
  FCC_A1
1.000000E-01      940.24
1.075000E-01      939.62
. . . . .
2.950000E-01     1084.87
```

After a successful calculation, you can go to the POST module to plot the T0 line against the stepping composition variable or another varying axis, or to impose the calculated T0 line onto a normal phase diagram [normally plotted as a T-x isopleth].

PARAEQUILIBRIUM (P)



See Console Mode examples 42 and 43.

This is an advanced option. Select **P** to calculate the paraequilibrium state between two specific phases (the *paraequilibrium lines*). It allows a stepping calculation of paraequilibrium lines where the chemical potential for one or more interstitial components (that are considered as back diffusion elements, such as C and N) but not for the other (s) in two partially equilibrated phases are equal.

More than one interstitial component can be treated as fast-diffusion species (such as C, N, O, S, etc., as individual or combined) in a paraequilibrium stepping calculation.



The composition condition for the interstitial components cannot be set as the stepping variable if you want to make this calculation.

To ensure a successful stepping calculation of paraequilibrium states between two specific phases in a defined alloy system, it is important to first make a starting-point equilibrium calculation with an initial overall composition in the current system. However, it is unnecessary to obtain an equilibrium in which either one or both of the target phases is stable.

The initial overall composition must have a reasonable setting for the desired paraequilibrium calculation for the two target phases. This is especially true where there is more than one interstitial component to be considered in the paraequilibrium state, because different interstitial components (for example C and N combined) may have significant different behaviours as partitioning into different structured phases; otherwise, for one chosen interstitial component the initial overall composition is OK for the paraequilibrium calculation between the specified two phases, but for other chosen interstitial component(s) it might be impossible to calculate the paraequilibrium state.

Always check if the chosen `phaseA` and `phaseB` have the exact same definition of elements and if the chosen interstitial components are all in the vacancy sublattice sites of the two phases; otherwise the program cannot find the paraequilibrium state (as it is impossible to correctly calculate u-fractions).

Always have a comprehensive understanding of the normal phase diagram for the currently investigated system, so that you make the appropriate choice of the phase pair and starting bulk composition for the system.

Always set the status of the chosen interstitial components as SPECIAL using the command:

```
CHANGE_STATUS COMPONENT <interstitial component> = SPECIAL
```

By doing this, you get a clear picture on u-fractions of various substitutional and interstitial components, which are different from the overall composition in the system. The SPECIAL status means that specified component(s) are not included in summations for mole or mass fractions. Therefore, all the composition variables plotted from the paraequilibrium calculations are u-fraction related quantities.

Always make a single-point paraequilibrium calculation by the command-sequence of `ADVANCED_OPTIONS → PARAEQUILIBRIUM`, prior to performing this `STEP → PARAEQUILIBRIUM` command-sequence, although this might not be always necessary for some systems.

With this stepping calculation specify the following:

Name of first phase: <Phase A>

Name of second phase: <Phase B>

The names of the two target phases A and B, between which the paraequilibrium states establish, must be typed at the above two prompts subsequently or on the same (first) line at once (separated by an empty space, e.g. `FCC BCC, FCC#2 M23C6`).



It is important to understand that this is the calculation of a paraequilibrium state between the two specified phases.

Particularly, there are these issues to consider:

1. Both chosen phases must have similar interstitial/vacancy sublattices where the fast-diffusion interstitial component(s) occupy.
2. The choice on the target phase pair must be reasonable for the defined system and specified initial overall composition.
3. Both target phases should have phase constitution definitions that cover all the defined substitutional and interstitial components of the current alloy system; or
4. It is impossible to calculate the paraequilibrium state between the target phase pairs with given interstitial component(s) in the currently defined system.

Fast diffusing component: `/C/: <Interstitial component(s)>`

Fast diffusing component: /None/: <Interstitial component(s)>

The name(s) of the fast-diffusing interstitial component(s) (C as the default single component) must be given either one by one at each of the above prompts subsequently or in a combination (separated by an empty space in between, e.g. C N S) at the same (first) prompt; otherwise, press <Enter> key to start the paraequilibrium line stepping-calculation.

Note the following:

Such specified fast-diffusing interstitial component(s) must be appropriately defined according to the phase constitution definitions of the two selected phases: These must be located on the interstitial/vacancy sublattices in both chosen phases.

If there is only one fast-diffusing component which is carbon, press <Enter> to accept the default value (C) at the first prompt; if the single fast-diffusing interstitial component is another element (e.g. N), appropriately type interstitial component the name at the first prompt;

If there are two or more fast-diffusing components (e.g. C and N), type their names at the above prompts subsequently or at the same (first) prompt (separated by an empty space, such as C N);

To finish the input of fast-diffusing elements, accept NONE at a repeated prompt;

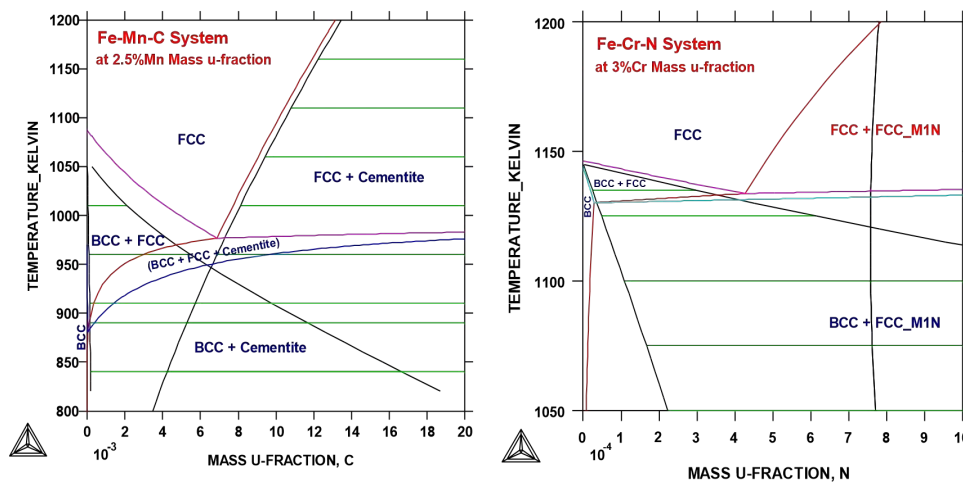
If NONE or a non-existing component name is typed at the first prompt, it means no back diffusion is to be considered, and the para-equilibrium calculation is thus cancelled entirely.

During the STEP → PARAEQUILIBRIUM calculation procedure, the calculated paraequilibrium states include the:

- corresponding stepping conditions (e.g. temperature in K, or the stepping composition variable of the matrix component or of one of substitutional components) which has already set as the stepping variable by the SET_AXIS_VAR command);
- amounts of the phase A in mole number [i.e. NP (phaseA)];
- amounts of the phase B in mole number [i.e. NP (phaseB)];
- contents of the interstitial component(s) in the phase A expressed in u-fractions [i.e. u-f (phaseA, component (s))];
- contents of the interstitial component(s) in the phase B expressed in u-fractions [i.e. u-f (phaseB, component (s))];
- LNACR (component) value(s) for the interstitial(s).

After a successful STEP → PARAEQUILIBRIUM calculation, you can go to the POST module to plot a paraequilibrium phase diagram, or to impose the calculated paraequilibrium states onto a normal phase diagram [normally plotted as a T–X isopleth with one of the considered interstitial component(s) as the x-axis variable].

However, the stepping calculation procedure for the currently specified paraequilibrium states between the two specified phases may find difficulties at some steps due to some possible numerical problems (normally regarding to the u-fractions of the interstitial components under some composition ranges), or it may completely fails. In the latter case, it implies that the chosen target phase pair may be unreasonable for the defined alloy system or for the defined initial overall composition, or one or both phases may have inappropriate phase constitution definitions regarding the specified interstitial component(s) and substitutional components. Then, you must either modify the settings of initial overall composition or specify the reasonable target phase pair with an appropriate choice of the fast diffusion interstitials in the defined alloy system.



The figure above shows the plot of a paraequilibrium calculation of isopleths: Formation of para-pearlite in two Fe-based alloys, with equilibrium results appended.



The calculated paraequilibrium phase boundaries (black lines) are shown with tie-lines (in green-colour). In the Fe-2.5Mn-C alloy system, C is considered as fast diffusing interstitial component in the BCC+FCC and FCC+Cementite paraequilibrium stepping calculations; while in the Fe-3Cr-N alloy system, N is treated as fast diffusing interstitial components in the BCC+FCC and FCC+FCC_M1N (i.e. FCC#1+FCC#2) paraequilibrium stepping calculations.



During a STEP calculation, the value of the stepping axis variable for each calculated equilibrium is listed and also the set of stable phases.



You can terminate the mapping of a line by pressing a single <Ctrl-A> (Windows) or <Ctrl-C> (Linux). This can be useful in order to stop a longish calculation without losing what is already calculated.

If there is any convergence problem in finding a stable solution at any stage during a calculation procedure enforced by a STEP_WITH_OPTIONS command-sequence, this message displays:

```
Convergence problems, increasing smallest site-fraction from 1.00E-30 to hardware
precision 2.00E-14. You can restore using SET-NUMERICAL-LIMITS
```

This implies that smallest site fraction in the current POLY3 workspace is automatically increased from the default value 1.00E-30 to the hardware-dependent precision (under Linux, as 2.00E-14). For other subsequent POLY-module calculation in the current TC run, you can use the POLY command SET_NUMERICAL_LIMITS to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

Complex miscibility gaps of various solution phases are automatically detected during a stepping calculation, and two or more composition sets for each of such solution phases are automatically generated as well, through an automatic Global Minimization Test procedure (by specifying a Global Test Interval value and confirming the Automatically add initial equilibria in the ADVANCED_OPTION STEP_AND_MAP command-sequence). As a particular case, such an automatic Global Minimization Test ensures that you can now start calculating from high temperatures in an austenitic steel (metallic FCC_A1 solution phase) where the MC carbides/nitrides/carbonitrides (i.e. the C-/N-rich sides of the FCC_A1 miscibility-gap, often (while not always) being referred to as FCC_A1#2, FCC_A1#3, etc.) are not stable, and during the MAP command the MC carbides/nitrides/carbonitrides may first become metastable with a composition different from the metallic FCC_A1 phase and later also stable.

Occasionally, it may be necessary to have a specified increment other than the default value for the defined stepping axis-variable, in order to calculate/plot a smoother property diagram.

To get a complete property diagram, sometimes (especially in some earlier Thermo-Calc versions) it may also be required to have more than one starting equilibrium-points (under another starting equilibrium condition), and repeat the stepping calculation over the same stepping axis-variable range (while without over-writing the same POLY3 workspaces via a SAVE_WORKSPACE command). However, using the current STEP procedure such a requirement become less necessary.

TABULATE



This command is available for a table entered in either the POLY or POST module.

For any entered table, this command gives a table of values from equilibria calculated with a STEP command.



Unlike the TAB module's command (also called TABULATE) it is not possible to plot columns from the tabulated tables. For this use normal POST commands.

| | |
|---------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | TABULATE |
| Prompts | Name: <Name of a table entered in either POLY or POST> Specify a table name that is entered in either the POLY or POST module. |
| | Output on screen or file /Screen/: Specify a file name if you want to save on a file the table values along the defined STEP calculation, or press <Enter> if want to see the table values displayed. |

Gibbs Energy System (GES) Commands

In this section:

| | |
|-------------------------------------------------|-----|
| ADD_COMMENT | 204 |
| AMEND_ELEMENT_DATA | 204 |
| AMEND_PARAMETER | 205 |
| Solution Models in the GIBBS (GES) Module | 207 |
| AMEND_SYMBOL | 218 |
| CHANGE_STATUS | 220 |
| ENTER_ELEMENT | 221 |
| ENTER_FUNCTION | 222 |
| ENTER_PARAMETER | 223 |
| About the ENTER_PHASE Command | 225 |
| ENTER_SPECIES | 230 |
| ENTER_SYMBOL | 231 |
| LIST_CONSTITUTION | 235 |
| LIST_DATA | 235 |
| LIST_PARAMETER | 236 |
| LIST_PHASE_DATA | 237 |
| LIST_STATUS | 237 |
| LIST_SYMBOL | 240 |
| READ_GES_WORKSPACE | 241 |
| READ_WORKSPACES | 241 |
| RECOVER_START_VALUES | 242 |
| REINITIATE | 242 |
| SAVE_GES_WORKSPACE | 243 |
| SAVE_WORKSPACES | 243 |

| | |
|------------------------|-----|
| SET_R_AND_P_NORM | 245 |
|------------------------|-----|

ADD_COMMENT



This command is for the Gibbs Energy System (GES) module.

Use the ADD_COMMENT command to add a comment or make notes about parameters.


AMEND_ELEMENT_DATA



This command is for the Gibbs Energy System (GES) module.

The data for an element (in the SER, the Stable Element Reference, state) can be changed by this command. It should only be used for the elements that do not have any data in the database because the element data available in the database is set by the database-developer for the purpose of internal consistency. Except for the mass, the other values have no influence on the calculations.

| Syntax | AMEND_ELEMENT_DATA |
|---------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | Element name: <Element name> Specify the name of the element for which you want to change the data. |
| | New stable element reference /ABCD/: <Name of ser> Press <Enter> to accept the default SER or specify a new SER for the element. Important: The default name should not be changed if this data is retrieved from a database. This name is used when parameters for a phase are listed and the database assumes that the stable element reference is the same as in the database. Only if the element's data have not been fetched from a database, e.g. entered manually, can you enter a new SER. |
| | New atomic mass /xx.xxxx/: <yyyyyy> Press <Enter> to accept the default atomic mass or specify a new value for the element. The atomic mass of the element is given in g/mol. |
| | New h(298.15)-h(0) /xxx.xxx/: <yyyyyy> Press <Enter> to accept the default H(298.15)-H(0) or specify a new value for the element. H(298.15)-H(0) is the enthalpy difference between 298.15 K and 0 K for the element in its SER state. |
| | New s(298.15) /xx.xxxx/: <yyyyyy> Press <Enter> to accept the default S(298.15) or specify a new value for the element. S(298.15) is the absolute value of the entropy at 298.15 K for the element in its SER state. |
| | Default element reference state symbol index /#/: <index> |

| Syntax | AMEND_ELEMENT_DATA |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <div>  <p>The index only changes the symbol, not any value. Normally the index is set correctly by the database. Only when manually entering data, you must set the index to get the correct symbol.</p> </div> <p>Specify an index for the default listing parameters (symbol), or press <Enter> to accept the pre-set index. 0 is for G, 1 is for H_{298} and 2 is for H_0.</p> <p>The index is to define the symbol printed in parameter listings. The symbol can be:</p> <ul style="list-style-type: none"> G the data are referred to Gibbs energy at a variable temperature (also called <i>lattice stability</i>). H_{298} the data are referred to the enthalpy of the element at 298.15 K and 1 bar. H_0 is the same as H_{298} but at the temperature 0 K. |

AMEND_PARAMETER



This command is for the Gibbs Energy System (GES) module.




There is also a PARROT module command with the same name.

Use this command to interactively change/amend the temperature-pressure function of a parameter. This is useful to correct typing errors because the old function is made available on the terminal for interactive editing.

► ["About the ENTER_PARAMETER Command" on page 264](#)

| Syntax | AMEND_PARAMETER |
|---------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Parameter: <Parameter name></p> <p>Specify a correct parameter name. If a parameter name is not acceptable or you only press <Enter>, the error message displays:</p> <p>Error, please re-enter each part separately</p> <p>The program prompts for separate input for each part for a parameter name.</p> |
| | <p>Identifier (/X/): <G or L, or TC, or BM, or V0 or VA or VC or VK></p> <p>Specify one of these legal identifiers as described for ENTER_PARAMETER.</p> |
| | <p>Phase name (/ABCD/): <Phase name></p> <p>Specify the phase name.</p> |
| | <p>Constituent (in sublattice # /ABC/): <Species name></p> <p>Specify the constituent name.</p> |

| Syntax | AMEND_PARAMETER |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>Interacting constituent (in sublattice # /xyz/): <Species name></p> <p>Specify the interacting constituent name: If there is no interacting constituent, press <Enter>.</p> |
| | <p>Interacting constituent (in sublattice # /xyz/): <Species name></p> <p>If there are more than one interacting constituents, specify them; otherwise press <Enter>.</p> |
| | <p>Degree /#/ : <Degree></p> <p>Specify a numerical number as the degree of the phase parameter.</p> |
| | <p>After the parameter name is specified correctly, the program lists its current definition (either present in the database or defined by the ENTER_PARAMETER command), such as:</p> <pre>L (PHASE2,AL,MG;1)= 298.15<T<2000.00: +5000 2000.00<T<4500.00: +4500 4500.00<T<6000.00: +4000</pre> <p>Then you are prompted to change the parameter definition, as shown below:</p> <p>Do you want to change the number of ranges /No/:</p> <p>Enter Y if you want to change the number of ranges for the chosen function, or change some of the temperature limits in the definition. Then retype both the low/high temperature limits and functions.</p> <p>If you do not want to change the number of ranges but want to change the function(s) in one or more ranges, press <Enter> to accept the default N, then the whole definition of the chosen parameter in all ranges (if any) is listed on screen, such as:</p> <pre>DIFFERENT FUNCTIONS IN THESE RANGES 298.15<T<2000.00 2000.00<T<4500.00 4500.00<T<6000.00</pre> <p>The prompt is given:</p> <p>Do you want to change range limits /No/:</p> <p>If there is more than one range, this question is prompted press <Enter>.</p> |
| | <p>Range number (0 to exit) /0/ : <Range number></p> <p>If the function of a parameter is different in two or more temperature ranges, you must specify the range of the function of which you want to amend. Or press <Enter> or type 0 to exit this command without making any changes.</p> |
| | <p>Function:</p> <p>The previous function is available for editing. The editing is performed within the general subroutine FOOLED, as described in "AMEND_SYMBOL" on page 218. This routine prompts as follows:</p> <pre>1:+:></pre> |

| Syntax | AMEND_PARAMETER |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>The prompt consists of the current position in the string and the character at that position between colons, (::).</p> <p>COMMANDS</p> <p>These commands can be given:</p> <ul style="list-style-type: none"> • Help: ? • Move CP to last or first character: <+/-> A • Delete characters from CP: <+-#characters> D • Exit: E • Find: <#occurrences> F<string>@ • Insert: I<string>@ • Move: <+-#positions> M • Restore string: R • Substitute: S<OLD>@<NEW>@ • Type string: T <p>Where CP denotes the current position in a string, # means number of, @ is a terminator of an input or search string.</p> <div>  <p>When the string is typed the character at the current position is replaced by an underscore _.</p> </div> <p>To finish the editing of the current function, type E at the prompt.</p> |

Solution Models in the GIBBS (GES) Module

▶ ["AMEND_PHASE_DESCRIPTION" on page 214](#)

The AMEND_PHASE_DESCRIPTION command is used to specify/amend phase descriptions if a phase has a miscibility gap, uses a special excess energy model, or has a specific additional contribution to its Gibbs energy, for example.

This topic outlines the application of each option and includes important information about each command.

There are many solution models implemented in the GIBBS module (type `INFO MODELS` to see details about various thermodynamic models). However, these are switched on and handled differently via various GIBBS routines/commands:

-
- The first models the non-ideality as excess parts, i.e. by amending the phase's EXCESS_MODEL and/or TERNARY_EXTRAPOLAT models.
 - The second models the non-ideality as ADDITIONAL parts, i.e. by amending the phase's other subjects in this command, e.g. MAGNETIC_ORDERING for the Magnetic Ordering Model, DISORDERED_PART for the CVM Approach in modelling chemical ordering/disordering phenomenon, QUASICHEM_IONIC for using a quasi-chemical entropy term for an ionic two-sublattice liquid solution phase, QUASICHEM_FACT00 or QUASICHEM_IRSID for describing a substitutional liquid solution phase, DEBYE_HUCKEL for the DHLL/SIT Model in describing a dilute aqueous solution phase, etc.
 - The third implements the model entirely or partially into the GIBBS module and related database(s), such as for the electrostatic contribution in an AQUEOUS solution phase by the Complete Revised_HKF Model, the Murngham Model, Birch-Murngham Model or Generalized PVT Model for high-pressure/temperature volume contribution in a solid or liquid phase, the SUPERFLUID Model for the non-ideal EOS and non-ideal mixing in a gaseous mixture.

NEW_CONSTITUENT

Use this if you want to add a new constituent to a phase. It is illegal to add new constituents to an ionic two-sublattice liquid phase.

RENAME_PHASE

Use this to change the names of some specific phases. For example, a phase called *FE3O4_S* may be better named *Magnetite* to help identify it during the calculations and postprocessing. This is also a way to delete a phase by hiding it under a new name.

SITE_RATIOS

Use this to change the number of sites (i.e. the stoichiometric coefficients of various sublattices) in a sublattice phase.

COMPOSITION_SETS

Use this for solution phases that may have miscibility gap(s). However, this is less important today and often unnecessary to define additional composition set(s), since the implemented Global Minimization Technique can usually detect and add such composition set(s) in an automatic manner where it is really necessary during equilibrium calculations (of single-points, stepping or mapping).

MAJOR_CONSTITUENT

Use this to set major constituent(s) on each sublattice in each composition set for a solution phase. This is useful to make calculations converge faster because it may simplify giving start values when calculating the equilibrium as those phases with miscibility gaps should have different major constituents for each composition set. The databases often set major constituents for several phases automatically when data are retrieved.

FRACTION_LIMITS

Use this to limit the application range (in terms of mole-fractions of all the involved elements) of a particular solution phase. This is useful to avoid automatic creations (enforced by the Global Minimization Technique) of additional composition sets for some solution phases (such as AQUEOUS solutions or dilute Fe-based liquid mixtures) of which the used models [e.g. the `SIT Model` or the `Complete Revised_HKF Model` for AQUEOUS solution, or the modified dilute solution parameters (plus a quadratic term, according to Hillert (1986) based on the SigworthElliot Model (Sigworth and Elliot, 1974) for Fe-rich liquid mixture] cannot be appropriately applied on a full scale.

Globally set the composition limits (in terms of mole fractions of various elements) in a specific solution phase, so that whenever the program finds a potential phase composition or a new composition set of possible miscibility gap(s) but that is out of this globally-set composition range, the program automatically ignores such a phase composition in an equilibrium calculation. This can be done either permanently inside a database (by enforcing this option for amending the phase-description of the solution phase) or temporarily within the GIBBS module (by using this phase-description amendment option).

This is important for solution phases for which the thermodynamic models and assessed data for the phases are for specific composition ranges, for example, the `FE_LIQUID` phase in the SLAG database is only applicable for Fe-rich liquid mixture, and the `AQUEOUS` phase in the TCAQ/PAQ and AQS/PAQS databases is only applicable for H₂O-dominant aqueous solution phase.

Specify the low and high mole-fraction limits for each of the elements possibly available within the considered phase (in the currently defined system, or in a certain database). Do this for all the possible elements (defined in the phase) in a single `AMEND_PHASE_DESCRIPTION FRACTION_LIMITS` command-sequence, for example:

```
TYPE_DEFINITION R GES AM_PH_DES FE_LIQUID FRACTION_LIMITS Fe 0 0.6
    Ag 0 0.01  Al 0 0.05  Ca 0 0.05  Co 0 0.01  Cr 0 0.01
    Cu 0 0.02  Mg 0 0.05  Mn 0 0.05  Mo 0 0.05  Nb 0 0.05
    Ni 0 0.05  Pb 0 0.05  Si 0 0.10  Sn 0 0.02  Ti 0 0.05
U 0 0.01  V 0 0.02  W 0 0.02  Zr 0 0.03
    B 0 0.01  C 0 0.01  H 0 0.01  N 0 0.01  O 0 0.01
```

DISORDERED_PART

This command is needed for the special treatment of chemically-ordered phases where the contributions from the disordered state are described by a phase without ordering sublattices (the disordered phase name must be specified).

Several checks are made that the ordered and disordered phases are compatible (sublattices, sites and constituents). A link is then created between the phases, and the disordered phase is hidden from application programs. The Gibbs energy for the ordered phase also includes the Gibbs energy for the disordered phase.

Phases which can have an order/disorder transformation have parameters split on two phases and are referred to as the *two phase* description in the GIBBS module. One of them has sublattices for chemical ordering, the other one represents the disordered state. Normally, the ordered BCC and FCC or HCP phases may have either 2 or 4 substitutional sublattice (plus one additional interstitial site), that are handled by the Two Substitutional-Sublattice Ordering Model or Four Substitutional-Sublattice Ordering Model, respectively.

Two phase means that the *ordered* phase has parameters that describe the ordering. The *disordered* phase has all parameters for the reference state and those for describing the disordered phase. The ordered phase may occur only in some systems whereas the disordered phase may occur frequently, typical examples are the disordered FCC and BCC which may become ordered as L12 or B2 in certain systems. In order to treat multicomponent systems where some subsystems have ordering it would be necessary to transform all parameters of BCC into a B2 model.

The parameters describing the disordered phase are not changed but the Gibbs Energy system is informed that the Gibbs Energy for the two phases should be added.

The method used calculates the Gibbs Energy of a two phase model with two or four substitutional sublattices for ordering.

$$G_m = G_m^{ord}(y'_i, y''_i) + G_m^{dis}(x_i) - G_m^{ord}(y'_i = x_i, y''_i = x_i)$$



The mole fractions x_i are calculated from the site fractions y_i . The last term means that the contribution from G_m^{ord} in a disordered state (same site fraction, equal to the mole fraction, on both sublattices) is subtracted. The effect of this is that the parameters in the ordered phase have no contribution to the disordered state.

MAGNETIC_ORDERING

Change the magnetic ordering parameter for a certain phase with magnetic ordering contribution, in terms of its anti-ferromagnetic factor. By default this is -1 for BCC phase and -3 for all other phases (FCC, HCP, etc.). The fraction value of the total enthalpy (due to short-range ordering above the magnetic transition temperature) is by default 0.40 for BCC phase and 0.28 for all other phases (FCC, HCP, etc.).

EXCESS_MODEL



See [example tcex52](#).

Use this to change the default Excess Model (for interaction energies) from the default (REDLICH-KISTER_MUGGIANU). The model handles the excess interaction energies in a solution phase is chosen from:

- REDLICH-KISTER_MUGGIANU: for binary (R-K) & ternary (R-K-M) interactions
- REDLICH-KISTER_KOHLER: for binary (R-K) & ternary (R-K-K) interactions
- FLORY-HUGGINS POLYMER MODEL: for interactions in a polymer mixture phase (F-H)
- MIXED-EXCESS-MODELS: (R-K default) for mixed binary excess model (R-K, Legendre & Polynom) of a substitutional solution phase
- HKF: for interaction in an AQUEOUS solution phase (HKF)
- PITZER: for interaction in an AQUEOUS solution phase (PIT)
- CENTRAL_ATOM_MODEL: for interaction in a liquid slag solution phase (C-A-M)

For extrapolations of excess energies from related binary systems to ternary or higher-order systems, the Redlich-Kister binary excess interaction parameters may be extrapolated with either a Muggianu extension (i.e. the default REDLICH-KISTER_MUGGIANU model) and a Kohler extension (i.e. the alternative REDLICH-KISTER_KOHLER model), where there is no ternary, quaternary or higher-order interaction parameter.



The REDLICHKISTER_KOHLER model is implemented only for ternary systems.

The MIXED-EXCESS-MODELS option works only for a substitutional phase with no sublattice (such as the metallic LIQUID phase) and it can be used to invoke asymmetrical simple or Legendre polynomial as binary excess energy models in addition to the default symmetrical Redlich-Kister model for the chosen pair of constituents in a substitutional phase with no

sublattice. Asymmetrical here means that the power series depend only on one of the constituents, for example with expansions based on the $[1-2 \cdot X(B)]$ term rather than $[X(A)X(B)]$.



Binary interaction parameters for such a pair of constituents must be entered prior to turning on the non-default Legendre or Polynom models.

TERNARY_EXTRAPOLAT



See [example tcex52](#).

Use this to change the extrapolation method from the default REDLICH-KISTER_MUGGIANU to another extrapolation model. This method extrapolates from binary to ternary (and higher-order) excess interaction parameters in a solution phase and is chosen from:

- MUGGIANU for Muggianu Extrapolation from R-K parameters
- TOOP-KOHLER for Toop-Kohler Extrapolation Model
- KOHLER-ALL for Kohler Extrapolation Model
- MUGGIANU_RESTOR for Muggianu-Restor Extrapolation Model



Only when all the relevant binary excess energies in the current solution phase are treated by the default Redlich-Kister Model (i.e. the Mixed-Excess-Model should have not been used), the MUGGIANU_RESTOR method for ternary extrapolations is equivalent to the Redlich-Kister_Muggianu Model, or the KOHLER-ALL method to the RedlichKister_Kohler Model.

The default ternary extrapolation method MUGGIANU_RESTOR applies to a solution phase as a whole, whatever the binary excess model(s) enforced to each of individual binary pairs in the phase. In case that all the binary pairs in the phase use the default binary excess model REDLICH-KISTER, then the ternary extrapolation method becomes the so-called Redlich-Kister_Muggianu Model (in short as R-K-M), for extrapolations from binary parameters to ternary (and higher-order) excess energy terms; when no ternary L parameter is entered for that, such a default R-K-M Model is always used.

The KOHLER-ALL ternary extrapolation method can be turned on also for a solution phase as a whole, whatever the binary excess model(s) enforced to each of individual binary pairs in the phase. In case that all the binary pairs in the phase use the default binary excess model.

REDLICH-KISTER, then the ternary extrapolation method becomes the so-called Redlich-Kister_Kohler Model (in short as R-K-K), for extrapolations from binary parameters to ternary (and higher-order) excess energy terms; when no ternary L parameter is entered for that, such an R-K-K Model is used.

The TOOP-KOHLER ternary extrapolation method is applied in a special way: for a specific ternary system (e.g. A-B-C) in a solution phase, specify which two constituents as the so-called Kohler constituents and the remaining constituent as the so-called Toop constituent on a given sublattice. If for the A-B-C ternary system you have specified A and B, or B and A, as the Kohler constituents (entered as the basis constituent and first interacting constituent) and C as the Toop constituent, only the A-B binary interaction parameters are used in accordance with the Kohler ternary extrapolation formula for A-B-C ternary interaction, while any other binary interaction parameters involving the Toop species C (i.e. of A-C and B-C binaries) are used in line with the Toop-Kohler ternary extrapolation formula (for the A-C-B and B-C-A ternary interactions).

DEBYE_HUCKEL

To use the DHLL (Debye-Hückel Limiting Law) model and SIT (Specific Ionic Interaction Theory) model for a dilute AQUEOUS solution phase, switch the DEBYE_HUCKEL part on, and it removes previously set (if any) ADDITIONAL part on the non-ideality for the chosen AQUEOUS phase.

HKF_ELECTROSTATIC

To use the hypothetical electrostatic contribution for the chosen phase (it must be an aqueous solution phase using the Complete Revised_HKF Model). It removes previously set (if any) ADDITIONAL part on the non-ideality for the chosen AQUEOUS solution phase.

QUASICHEM_IONIC

To use the Quasichemical-Ionic model for the chosen liquid phase, you must have already entered/retrieved a liquid phase as an ionic two-sublattice liquid solution phase (normally, that is the IONIC_LIQ phase), and then use this amending option to switch QUASICHEM_IONIC on. It creates a completely new liquid solution phase [namely the QUAS_IONIC phase which uses the Quasichemical Model for the entropy, according to Mats Hillert (2001: *J of Alloys and Compounds*, 320, 161-176)], while the original IONIC_LIQ phase remains in the system and is not changed by this option.

QUASICHEM_FACT00

To use the Quasichemical Model developed by Kongoli et al. (1998)¹, you must have entered/retrieved a liquid phase using a normal substitutional liquid model with specified associates or species (on a single lattice site), and then turn on the option QUASICHEM_FACT00. This removes the previously-set (if any) ADDITIONAL part on the non-ideality for the chosen liquid phase.



See example [tcex49](#).

QUASICHEM_IRSID

To use the Kapoor-Frohberg-Gaye Quasichemical Cell Model (i.e. the Quasichemical Model developed by IRSID, France) for a liquid SLAG solution phase, you can use a normal liquid model with specified associates or species.

GLASS_TRANSITION

To use the special model for glass transition of a liquid phase. It removes previously set (if any) ADDITIONAL part on the non-ideality for the chosen liquid phase.

REMOVE_ADDITION

To remove all the selected ADDITIONAL part from the Gibbs energy description for the chosen phase. If preferred, set a specific phase-status bit for a phase, use the PHASE_BITS option as long you know the restrict meaning of each part of a phase- status bits.

DEFAULT_STABLE

Set phases as default-stable, which helps you to have a better guess of which phases that should be stable at the first calculation.

AMEND_PHASE_DESCRIPTION





This command is for the Gibbs Energy System (GES) module.



Also see "[Solution Models in the GIBBS \(GES\) Module](#)" on page 207 for detailed information about this command and its options.


Specify/amend phase descriptions if a phase has a miscibility gap, uses a special excess energy model, or has a specific additional contribution to its Gibbs energy, for example.

1. Kongoli, Florian, Arthur D Pelton, and Yves Dessureault. 1998. "Thermodynamic Modeling of Liquid Fe-Ni-Cu-Co-S Mattes." Metallurgical and Materials Transactions B 29 (3): 591–601. doi:10.1007/s11663-998-0094-y.

| Syntax | AMEND_PHASE_DESCRIPTION |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Phase name: <Phase name></p> <p>Specify the name of the phase.</p> <p>Amend what /Composition_Set/: <Subject></p> <p>Several subjects for the phase can be amended but most often this command is used to enter two or more composition sets for a phase. If a phase has a miscibility gap it is necessary to have two composition sets, one for each possible composition that can be stable simultaneously.</p> <p>Enter a question mark at the prompt to get a list of all possibly amended subjects for a phase.</p> |
|  | <p>There are no additional prompts for DEBYE_HUCKEL, HKF_ELECTROSTATIC, GLASS_TRANSITION, QUASICHEM_FACT00, QUASICHEM_ISRID, REMOVE_ADDITION, and DEFAULT_STABLE.</p> |
| RENAME_PHASE | <p>New phase name /ABCD/: <Phase name></p> <p>Give a new phase name for the chosen phase, or press <Enter> to keep the default shown.</p> |
| Site_ratios | <p>Sites in first sublattice /XX/ : <YY> Sites in second sublattice /XX/ : <YY></p> <p>Specify the site numbers for each of the prompted sublattices for the current phase. Press <Enter> to accept the previous definitions.</p> |
| New_constituent | <p>Sublattice /#/: <Sublattice number></p> <p>Specify the sublattice where the new constituents are located.</p> <p>Species: <Species name></p> <p>Give a valid species name.</p> |
| Composition_sets | <p>New highest set number /#/: <Set number n></p> <p>The default value (#) is usually one higher than the current value. All phases have initially one composition set. If a lower value (i.e. lower than the default one) is given, that specific composition sets are deleted.</p> <p> You cannot take away the first composition set.</p> <p>Major constituent(s) for sublattice #: /AB/: <Major constituent(s)></p> <p>Specify the new major constituent(s) for the sublattice #, or press <Enter> to accept the default which was automatically set according to the specified composition set of the phase.</p> <p>This prompt is repeated for all available sublattices in the chosen phase. The major constituents in each sublattice can be given. This may simplify giving start values when calculating the equilibrium as phases with miscibility gaps should have different major constituents for each composition set.</p> |
| Major_constituent | <p>Composition set /1/: <Composition set number></p> |

| Syntax | AMEND_PHASE_DESCRIPTION |
|--------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>Give the composition set (digit number) for the chosen phase, or press <Enter> if you want to set major constituents for the specified composition set.</p> <p>Major constituent(s) for sublattice #: /AB/: <Major constituent(s)></p> <p>Specify the new major constituent(s) for the sublattice #, or press <Enter> to accept the default which is automatically set according to the specified composition set of the phase.</p> <p>This prompt is repeated for all available sublattices in the chosen phase for the specified composition set.</p> <p>The major constituents in each sublattice can be specified. This is useful in order to make calculations converge faster and more easily (because it may simplify giving start values when calculating the equilibrium as those phases with miscibility gaps should have different major constituents for each composition set). The databases often set major constituents for several phases automatically when data are retrieved.</p> |
| Fraction_ limits | <p>Element : <el1></p> <p>Low fraction limit /0/ : <Appropriate low limit></p> <p>High fraction limit /1/ : <Appropriate high limit ></p> <p>Element : <el2></p> <p>Low fraction limit /0/ : <Appropriate low limit></p> <p>High fraction limit /1/ : <Appropriate high limit></p> <p>Element : <eln></p> <p>Low fraction limit /0/ : <Appropriate low limit></p> <p>High fraction limit /1/ : <Appropriate high limit ></p> |
| Magnetic_ ordering | <p>The antiferromagnetic factor /XX/: <YY></p> <p>Specify the anti-ferromagnetic factor for the chosen phase. This should be –1 for BCC phase and –3 for all other phases (FCC, HCP, etc.).</p> <p>Short range order fraction of the enthalpy /XX/: <YY></p> <p>The magnetic ordering is a second-order transformation and part of the enthalpy due to this transformation is due to short-range order. This value is the fraction of the total enthalpy that is due to short-range ordering above the magnetic transition temperature.</p> <p>The default value (xx) is 0.40 for BCC phase, and 0.28 for all other phases (FCC, HCP, etc.).</p> |
| Disordered_ part | <p>Disordered phase name: <Phase name></p> <p>Give the disordered phase name for which there is no ordering sublattice.</p> |
| Excess_model | <p>Model name /ABCDEFG/: <Model name></p> <p>The default model is the pre-set model for the solution phase, normally the REDLICH-KISTER_MUGGIANU model, or choose another model for the phase to be amended:</p> <ul style="list-style-type: none"> • REDLICH-KISTER_MUGGIANU • REDLICH-KISTER_KOHLER • FLORY-HUGGINS POLYMER MODEL |

| Syntax | AMEND_PHASE_DESCRIPTION |
|--------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <ul style="list-style-type: none"> • MIXED-EXCESS-MODELS (R-K default) • HKF • PITZER • CENTRAL_ATOM_MODEL <p>The MIXED-EXCESS-MODELS option has sub-options:</p> <p>First (the independent) constituent: <Constituent name></p> <p>Second (the dependent) constituent: <Constituent name></p> <p>Specify the binary pair of constituents in the current substitutional solution phase (the first one as the so-called independent constituent, and the second one as the dependent constituent), for which you wish to change the binary excess model from the default REDLICH-KISTER model to another model (LEGENDRE or POLYNOM).</p> <p>You are prompted with the first sub-option (i.e. <i>First (the independent) constituent</i> after you have specified the desired binary Excess model type. To make further changes of binary excess model for other specific binary pairs in the current substitutional solution phase, press <Enter> (implying that there are no more changes of binary excess model for all other possibly-remaining binary pairs that shall still use the default REDLICH-KISTER model).</p> <p>Excess model type: /Legendre/: <Desired binary excess model type></p> <p>For the currently-specified binary pair, choose one the legal binary excess models: LEGENDRE, POLYNOM or REDLICH-KISTER. If the default binary excess model REDLICH-KISTER is used for a certain binary pair, you can either specify the model name (or in short as R-K) or press <Enter>. After this sub-option, it returns to the first sub-option <i>First (the independent) constituent</i>: either for further change(s) of binary excess model of any other binary pair(s) or for termination (by pressing <Enter>) in the MIXED-EXCESS-MODELS option.</p> |
| Ternary_extrapolat | <p>Extrapolation method: /Toop-Kohler/: <Ternary model></p> <p>Choose a ternary extrapolation model for the current solution phase:</p> <ul style="list-style-type: none"> • TOOP-KOHLER for Toop-Kohler Extrapolation Model • KOHLER-ALL for Kohler Extrapolation Model • MUGGIANU_RESTOR for Muggianu-Restor Extrapolation Model <p>The TOOP-KOHLER option further prompts:</p> <p>Constituent in sublattice #: <Basis constituent name></p> <p>First interaction constituent: <Interacting constituent name></p> <p>Toop constituent: <Toop constituent name></p> <p>Specify the so-called Kohler constituents (entered as the basis constituent and first interacting constituent) and Toop constituent on a given sublattice in the current solution phase.</p> |
| Quasichem_ionic | <p>To use the Quasichemical Model for the chosen liquid phase, you must first enter it as an ionic liquid phase, and then use this amending option. It creates a completely new phase, the original IONIC_LIQUID phase remains in the system and is not changed.</p> |

| | |
|-------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | AMEND_PHASE_DESCRIPTION |
| | <p>Number of bonds/atom /2/: <Number of bonds per atom></p> <p>Specify the Z value (number of bonds per atom).</p> |
| Status_bits | <p>Correct the phase status bits. It is important to fully understand this command before using it:</p> <p>New status word (in hexadecimal) /04204000/: <New status bits></p> <p> "LIST_STATUS" on page 237</p> <p>Normally, these should never be changed in this way, because such phase status bits are automatically set on when all the phase descriptions (predefined in databases and amended in the GIBBS module) are defined properly. The only exceptions are for the Kapoor-Frohberg-Gaye cell model for liquid SLAG solution phase, which can be set only as 04208000; and for the complete Revised HKF AQUEOUS solution model, which can be set as 02084000.</p> |

AMEND_SYMBOL



This command is for the Gibbs Energy System (GES) module.



The same command is also available for the PARROT module.

Interactively calculate the current values of a function or table (predefined by the switched database or previously entered with ENTER_SYMBOL) at the current temperature and pressure condition, and also possible to modify the definitions of variables or functions.




The current values of the temperature and pressure used to calculate the functions or tables are the ones listed with LIST_STATUS. There is no way to change the current temperature and pressure values interactively.

To modify the definitions of entered symbols (variable, functions or parameters), the performance of this command is slightly different one from another, as described below:

- For variables, the values can be changed.
- For functions the low and high temperature limits in various ranges (if any), as well the expressions, can be changed.
- For parameters the low and high temperature limits in various ranges (if any), as well the expressions, can be changed.

| | |
|---------|---------------------|
| Syntax | AMEND_SYMBOL |
| Prompts | Name: <Symbol name> |

| Syntax | AMEND_SYMBOL |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>Specify the name of an entered symbol.</p> <p>For tables and functions (or parameters which are treated as functions after these are entered by the ENTER_SYMBOL command with the <code>Parameter</code> keyword, but not by the ENTER_PARAMETER command), after the symbol name is specified here, the program automatically calculates the values under the current temperature and pressure conditions, and lists the current values, such as:</p> <pre>FUNCTION VALUE 2.52500000E+01 TABLE VALUE 1.56000000E+02</pre> <p>For variables and functions (or parameters), there are additional prompts and depend on the symbol type.</p> |
| | <p>For a variable, its current value is displayed, and you can change it to a new value:</p> <pre>Value /Current value/: <New value></pre> <p>For a function (or a parameter entered as a symbol):</p> <pre>Do you want to change the number of ranges /No/:</pre> <p>Enter Y to change the number of ranges for the function, or change some of the temperature limits in the definition, then retype both the low/high temperature limits and functions (see all the remaining details in the ENTER_SYMBOL command.</p> <p>If you do not want to change it, press <Enter>. The definition of the chosen function in all ranges (if any) is listed, for example:</p> <pre>DIFFERENT FUNCTIONS IN THESE RANGES 298.15<T<2000.00 2000.00<T<4500.00 4500.00<T<6000.00</pre> <p>and this message displays:</p> <pre>Do you want to change range limits /No/:</pre> <p>If a function is different in two or more temperature ranges, you must specify the range of the function of which you want to amend. Or press <Enter> or type 0 to exit this command without making any change.</p> |
| | <pre>Range number (0 to exit) /0/: <Range number></pre> <p>Function:</p> <p>The previous function is available for editing. The editing is performed within the general subroutine FOOLED. This routine prompts as follows:</p> <pre>1:::></pre> <p>The prompt consists of the current position in the string and the character at that position between colons (::).</p> <p>COMMANDS</p> |

| Syntax | AMEND_SYMBOL |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>These commands can be given:</p> <ul style="list-style-type: none"> • Help: ? • Move CP to last or first character: <+/-> A • Delete characters from CP: <+--#characters> D • Exit: E • Find: <#occurrences> F<string>@ • Insert: I<string>@ • Move: <+--#positions> M • Restore string: R • Substitute: S<OLD>@<NEW>@ • Type string: T <p>Where CP denotes the current position in a string, # means number of, @ is a terminator of an input or search string.</p> <div>  <p>When the string is typed the character at the current position is replaced by an underscore _.</p> </div> <p>To finish the editing of the current function, type E at the prompt.</p> |

CHANGE_STATUS



This command is for the Gibbs Energy System (GES) module.

The status of an element or species or phase can be either ENTERED or SUSPENDED. The suspended status can be either implicit or explicit. The implicitly suspended status can be set e.g. for a species if any of the elements in its chemical formula is explicitly suspended. A species that is implicitly suspended becomes entered automatically if all its elements are set entered. After this command, a message shows which elements/species/phases are suspended or restored (entered). Consequently, the status bits for the specified elements or species or phases are changed, as listed with LIST_STATUS.

| Syntax | CHANGE_STATUS |
|---------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>For Element, Species or Phase /Species/: <Keyword></p> <p>Specify the keyword (element, species or phase).</p> |
| | <p>Suspend /Y/:</p> <p>By default the status is changed from ENTERED to SUSPENDED.</p> <p>If an element is suspended all species with this element become implicitly SUSPENDED too. A phase may become implicitly suspended if all its constituents or all constituents in a sublattice are</p> |

| | |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | CHANGE_STATUS |
| | suspended. |
| | <p>List of elements/species/phases: <Name of elements or species or phases></p> <p>Specify the names or indices of those elements or species or phases that shall become suspended or active. For names, these should be separated by a space and terminated with a semicolon (;) or an empty line. For indices it is possible to give a range by separating two numbers by a hyphen (-). The list should be terminated by a semicolon (;). Example: 5 1 7-12 FE;</p> |


ENTER_ELEMENT

Specify a system interactively. The program searches the currently switched or preset database for data for the given elements. The data for the elements in the database are the:

- mass in g/mol
- name of the Selected Element Reference State (SER) which normally is the stable phase for the element at 298.15 K
- enthalpy difference for the element in the SER state at 298.15 K and zero K
- absolute entropy for the element in the SER state at 298.15 K.

The two predefined elements, i.e. electrons and vacancies, have the chemical symbols /- and v_A, respectively. Initially, these are suspended but can be entered either by this command or CHANGE_STATUS.

If an aqueous solution phase is involved, in the GIBBS module you enter a special aqueous electron called, ZE. This is specially designed for appropriately calculating the standard electric potential in the aqueous solution system.

| | |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | ENTER_ELEMENT |
| Prompt | <p>Element name: <Element name></p> <p>Specify several elements on one line. The name of an element is its chemical symbol. The chemical symbols must be separated by spaces. Fictitious element names are legal but naturally no data are found in the database for them.</p> |
| |  <p>An element name (maximum 2 characters) can either have its first letter in upper and the second (if any) in lower case (i.e. Lower Case Mode) or both letters can be in upper or lower case (i.e. Upper Case Mode). The Upper or Lower Case Mode is selected by the command REINITIATE, which removes all data, and should be executed before any other command.</p> |

ENTER_FUNCTION



This command is available with the GES and TAB modules.

Used to define a new thermodynamic function to be included in the sixth column of tabular output. The last entered function is listed in the 6th column of all tables, and can be plotted (if choosing the Plot Column value 6) in all graphs, for all subsequently tabulated substances or reactions.

| Syntax | ENTER_FUNCTION |
|---------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | Name: <Name> Function: <Definition> |
| | A limited number of state variables, G, H, S, T, P, V and H298 can be used in the function definition. For example, $-(G-H)/T$ can be defined as a function which is identical to S for a substance or ΔS for a reaction, $G+T*S-P*V$ can be defined as a function which is U (internal energy) for a substance or ΔU (internal energy change) for a reaction. |
| Options | Name of the function (maximum 8 characters) and Definition of the function. A long function can be typed over several lines. A function should be terminated by a semicolon (;) or an empty line. |

EXAMPLE OUTPUT

For the pure substance Fe (using the SSUB database), by entering a function as $G+T*S-P*V$, the following table is obtained by typing <Enter> in the prompt `Output file /Screen/:`, and the figure by typing 6 in the prompt `Plot column /2/:`

```
TAB: ENTER-FUNCTION
Name: InEnergy
Function: G+T*S-P*V;
TAB: TABULATE_SUBSTANCE
Substance (phase): Fe
Pressure /100000/: <Enter>
Low temperature limit /298.15/: <Enter>
High temperature limit /2000/: <Enter>
Step in temperature /100/: <Enter>
Output file /try1/: try2
Graphical output? /Y/: <Enter>
Plot column? /2/: 6
```

This gives the following output:

OUTPUT FROM THERMO - CALC

Column 6: InEnergy G+T*S-P*V

Phase : FE_S

Pressure : 100000.00

Specie: FE

| T | Cp | H | S | G | InEnergy |
|-----------------------|-------------|-------------|-------------|--------------|----------------|
| (K) | (Joule/K) | (Joule) | (Joule/K) | (Joule) | |
| ***** | | | | | |
| 298.15 | 2.48446E+01 | 2.17972E-06 | 2.72800E+01 | -8.13353E+03 | 2.17972E-06 |
| 300.00 | 2.48905E+01 | 4.60049E+01 | 2.74338E+01 | -8.18414E+03 | 4.60049E+01 |
| 400.00 | 2.71299E+01 | 2.64957E+03 | 3.49085E+01 | -1.13138E+04 | 2.64957E+03 |
| 500.00 | 2.93561E+01 | 5.47211E+03 | 4.11976E+01 | -1.51267E+04 | 5.47211E+03 |
| 600.00 | 3.19293E+01 | 8.53245E+03 | 4.67701E+01 | -1.95296E+04 | 8.53245E+03 |
| 700.00 | 3.50985E+01 | 1.18777E+04 | 5.19207E+01 | -2.44667E+04 | 1.18777E+04 |
| 800.00 | 3.92042E+01 | 1.55830E+04 | 5.68623E+01 | -2.99068E+04 | 1.55830E+04 |
| 900.00 | 4.49645E+01 | 1.97726E+04 | 6.17903E+01 | -3.58387E+04 | 1.97726E+04 |
| 1000.00 | 5.42147E+01 | 2.46891E+04 | 6.69619E+01 | -4.22728E+04 | 2.46891E+04 |
| 1100.00 | 4.55851E+01 | 2.99025E+04 | 7.19412E+01 | -4.92328E+04 | 2.99025E+04 \$ |
| Stable phase is FE_S2 | | | | | |
| 1200.00 | 3.40840E+01 | 3.51037E+04 | 7.64466E+01 | -5.66322E+04 | 3.51037E+04 |
| 1300.00 | 3.49398E+01 | 3.85549E+04 | 7.92086E+01 | -6.44162E+04 | 3.85549E+04 |
| 1400.00 | 3.57994E+01 | 4.20918E+04 | 8.18293E+01 | -7.24692E+04 | 4.20918E+04 |
| 1500.00 | 3.66636E+01 | 4.57149E+04 | 8.43287E+01 | -8.07780E+04 | 4.57149E+04 |
| 1600.00 | 3.75330E+01 | 4.94247E+04 | 8.67226E+01 | -8.93314E+04 | 4.94247E+04 \$ |
| Stable phase is FE_S3 | | | | | |
| 1700.00 | 4.05217E+01 | 5.41173E+04 | 8.95609E+01 | -9.81363E+04 | 5.41173E+04 |
| 1800.00 | 4.12595E+01 | 5.82055E+04 | 9.18975E+01 | -1.07210E+05 | 5.82055E+04 \$ |
| Stable phase is FE_L | | | | | |
| 1900.00 | 4.60000E+01 | 7.74165E+04 | 1.02377E+02 | -1.17099E+05 | 7.74165E+04 |
| 2000.00 | 4.60000E+01 | 8.20165E+04 | 1.04736E+02 | -1.27456E+05 | 8.20165E+04 |

ENTER_PARAMETER



This command is for the Gibbs Energy System (GES) module.





There is also a PARROT module command with the same name.



["About the ENTER_PARAMETER Command" on page 264](#)

Use this command to enter TP-function(s) for a specific parameter for a phase interactively with this command. If there is already a parameter expression defined (for this parameter), that is deleted and replaced with newly entered one.

The entered TP-Function(s) for the parameter can be changed later with the command AMEND_PARAMETER.

| Syntax | ENTER_PARAMETER |
|-------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Parameter: <Parameter name></p> <p>As explained in "About the ENTER_PARAMETER Command" on page 264, specify a correct and complete Parameter Name, which should contain all the necessary parts of the general form:</p> <p><Identifier>(<Phase>,<Constituent array>;<Digit>)</p> <p>If a parameter name is not acceptable or <Enter>, is pressed, a message displays:</p> <p>*** Error, please re-enter each part separately</p> <p>and you are prompted for input for each required part for a parameter name.</p> |
| Options | Description or Information |
| Identifier | <p>Identifier (/X/): <G or L, or TC, or BM, or V0 or VA or VC or VK></p> <p>If this command is used one or more times, the previous value on this prompt is set as default. Press <Enter> for the same type identifier or specify a new type.</p> |
| Phase name | <p>Phase name (/ABCD/): <Phase name></p> <p>Each parameter is valid for a specific phase only. The name of that phase must be supplied (maximum 24 characters). The name can be abbreviated.</p> |
| Constituent | <p>Constituent (in sublattice # /ABC/): <Species name></p> <p>A parameter is identified by the constituents on a specified sublattice site of the given phase, the stoichiometric coefficients of which are multiplied with the parameter. The name of the constituent can be abbreviated.</p> <div>  <p>It is the species name, not the stoichiometric formula required here.</p> </div> <p>If this command is used one or more times, the previous value on this prompt is set as default. Accept it by pressing <Enter> if the constituent is the same, or specify a new species name.</p> |
| Interacting constituent | <p>For phases with several sublattices, the program asks for one constituent in each sublattice.</p> <p>Interacting constituent (in sublattice # /XYZ/): <Species name></p> <p>If this command is used one or more times, the previous value on this prompt is set as default. Press <Enter> to accept it if the constituent is the same, or specify a new species name.</p> <div>  <p>To cancel the default value of the interacting constituent type NONE or the name of another constituent.</p> </div> <p>This question is repeated until all the interested interacting constituent(s) on a specific</p> |

| Syntax | ENTER_PARAMETER |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>sublattice in the phase are specified, and finally an <Enter> is enforced.</p> |
| Degree | <p>Degree /#/ : <Degree></p> <p>Degree is model-dependent. Specify an integer number (a value from 0 through 9) as the degree of composition-dependent interaction contribution for the phase parameter. This is valid for excess energy (L), Curie temperature (T_C) and Bohr magneton number (B_{MAGN}), as well as for volume-related parameters (V_0, V_A, V_C or V_K).</p> <p>For binary interaction parameters, the degree is usually the power in the Redlich-Kister expression. For ternary interaction parameters, it is usually the Hillert ternary index.</p> <p>For a standard G parameter for a pure component (end-member) its degree should be always 0 and this prompt should not display.</p> |
| Phase parameter | <p>After this prompt, the program echoes on the screen the full TP-Function of the phase parameter.</p> <p>Low temperature limit /298.15/ : <Lowest temperature limit in K></p> <p>Specify the lowest temperature limit (in Kelvin), or the lowest-pressure limit (in Pascal but entered as a negative number), for the current TP-Function.</p> <p>Function: <Definition for a function></p> <p>A TP-Function consists of terms in T and P.</p> <p>& <Continuation of the definition for the current function></p> <p>Continuation of a TP-Function definition.</p> <p>High temperature limit /6000/ : <High temperature limit in K></p> <p>Specify the high temperature limit (in Kelvin), or the high-pressure limit (in Pascal; only if the <i>lowest limit</i> is entered as a negative number) for the current TP-Function.</p> <p>Any more ranges? /N/ :</p> <p>Enter Y for more function(s) or N to end this command.</p> |

About the *ENTER_PHASE* Command

► ["ENTER_PHASE" on page 228](#)

With the command ENTER_PHASE, the phase name, phase-type, sublattice number, and constituents or constituent array(s) for the phase are entered into the GIBBS workspaces.

ABOUT PHASE NAMES

A thermochemical system must have at least one phase (which is a homogeneous part of the system with a uniform composition and structure). In the GIBBS module, any number of

phases can be entered for a system and for each phase there must be a description of how its Gibbs energy varies with temperature, pressure and composition. A phase has a large amount of data connected to it, e.g. it starts with a phase name:

- It may be treated as a special phase-type;
- It may have structural information about sublattice(s), etc.,
- There must be a list of constituents (for a substitutional phase with no sublattice) or of constituent arrays (for a sublattice phase);
- There may be basic information on what kind of EXCESS_MODEL (polynomial expression) is used to describe the binary, ternary and/or higher-order interactions between constituents;
- There may be so-called Additional contributions to the Gibbs energy of the phase from special physical phenomena, e.g. magnetic ordering, hypothetical electrostatic interaction, and so forth;
- There must exist all the parameters required for the descriptions of thermochemical properties (i.e. G terms for standard Gibbs energies, and L terms for binary, ternary or higher-order interaction excess energies) and of some special physical properties (e.g. the Curie temperature T_C and Bohr magneton number B_{MAGN} (or B_M) for magnetic ordering, V_0 - V_A - V_C - V_K parameters for volume contributions, Born functions for hypothetical electrostatic interaction in an aqueous solution phase) stored in connection with the phase.

ABOUT PHASE TYPE CODE

A G phase (gaseous mixture) or an A phase (aqueous solution) is usually treated as a substitutional phase without sublattice, and that an L phase (ordinary liquid solution) is normally (but not always) modelled as a substitutional phase without sublattice, too.

The F and B phase-types are useful for ordered FCC (or HCP) and BCC solution phases handled by the so-called Four Substitutional-Sublattice Ordering Model, which always requires that the solution phase must have four sublattices for substitutional ordering and can additionally have an interstitial sublattice.

For ordered FCC or HCP phases, these four substitutional sublattices represent four corners of the regular tetrahedron on these lattices all of which are the nearest neighbours. A *Normal 4-Sublattice Model* requires that all the G parameters for each of end-members with the same elements but distributed on different sites be given separately. However, as these corners are identical lattice points, the phase-type option F means that the G parameters need be given only once. The possible permutations are handled automatically. To be more clarified: An A-B binary solution phase (with the element A locates on one sublattice site and

B on three sublattice sites) treated by the Normal 4-Sublattice Model has to have 4 G parameters for 4 end-members, i.e. $G(\text{phase}, A:B:B:B)$, $G(\text{phase}, B:A:B:B)$, $G(\text{phase}, B:B:A:B)$ and $G(\text{phase}, B:B:B:A)$, because of that in the general case these G parameters can be different from each other. But for the FCC and HCP orderings, these are identical and thus all G parameters of such end-members need be given only once, and the possible permutations are then automatically handled by the GIBBS module. This significantly simplifies the usage of this model (*Four Substitutional-Sublattice Ordering Model*) in multicomponent alloys.

There are restrictions on the excess parameters allowed with the phase-type option F. You can only have excess parameters of these types:

$L(\text{phase}, A, B: *: *: *: 0 \dots 9)$

$L(\text{phase}, A, B:C, D: *: *: 0 \dots 9)$

The asterisk * means that the interaction parameter is independent on the constituents on its corresponding sublattice. No ternary interaction parameters (i.e. with three elements on one sublattice site) are allowed. The reason for this restriction is that it would be too complicated to handle all possible permutations. In the current *Four Substitutional Sublattice Ordering Model*, the binary interaction between A and B atoms is thus independent of the constituents on the other sublattices, where there are many other parameters to model the composition-dependence of the Gibbs energy (both in the ordered and disordered parts of the phase). The model for these ordered phases are always partitioned in a disordered part (with a single substitutional sublattice) and an ordered part (with four substitutional sublattices for ordering).

For ordered BCC phases, the phase-type option B means the same thing but the situation is more complicated, as the 4-sublattice ordering phase represents an irregular tetrahedron with two pairs of sites that are next nearest neighbours. Thus, for an A-B binary solution phase (with the element A locates on two sublattice site and B on other two sublattice sites) treated by the Normal 4-Sublattice Model, the end-member described by the $G(\text{phase}, A:A:B:B)$ term has four nearest neighbour bonds between A and B atoms, whereas the end-member described by the $G(\text{phase}, A:B:A:B)$ term has two nearest neighbour bonds between A and B atoms and two next nearest neighbour bonds



For detailed reference visit the Crystal Lattice Structure web page
<https://www.nrl.navy.mil/mstd/6390>.

The first end-member (described by the $G(\text{phase}, A:A:B:B)$ term) represents B2- ordering and the second (described by the $G(\text{phase}, A:B:A:B)$ term) stands for B32-ordering. There are two permutations of the $G(\text{phase}, A:A:B:B)$ term and four permutations of the $G(\text{phase}, A:B:A:B)$ term, automatically conducted in the Four Substitutional-Sublattice Ordering Model. And there are also two kinds of reciprocal interaction parameters, i.e.

$L(\text{phase}, A, B:C, D: *: *: 0 \dots 9)$ $L(\text{phase}, A, B: *: *: C, D: *: 0 \dots 9)$

An advanced feature with the phase-type options F and B is that a composition set that represents the solution phase has a suffix (indicating that it is really as an ordered or disordered phase) that is automatically added to its phase name in some listings of equilibrium calculations (when performing either single-point or stepping or mapping calculations, and when plotting the calculated property diagrams or phase diagrams). Such suffix indications can be:

- `_L12` or `_L10` for ordered FCC
- `_A1` for disordered FCC
- `_B2`, `_B32`, `_D03` or `_L21` for ordered BCC
- `_A2` for disordered BCC
- `_D019` and `_B19` for ordered HCP
- `_A3` for disordered HCP

| Solution Phase | Suffix for Disordered Phase | Suffix for Ordered Phase |
|----------------|-----------------------------|--------------------------|
| FCC PHASE | PHASE_A1 | PHASE_L12 |
| | | PHASE_L10 |
| BCC PHASE | PHASE_A2 | PHASE_B2 |
| | | PHASE_B32 |
| | | PHASE_D03 |
| | | PHASE_L21 |
| HCP PHASE | PHASE_A3 | PHASE_D019 |
| | | PHASE_B19 |


ENTER_PHASE



See ["About the ENTER_PHASE Command" on page 225](#) for details about the phase-type and other prompts.

With this command, the phase name, phase-type, sublattice number, and constituents or constituent array(s) for the phase are entered into the GIBBS workspaces. However, for the remaining parts of thermodynamic descriptions (i.e. thermochemical and physical parameters, excess model, and possibly additional contribution term) for the phase, the GIBBS commands `ENTER_PARAMETER` and `AMEND_PHASE_DESCRIPTION`, should be used sequentially.

Normally, data for a system are retrieved from the preset database after the elements and species are specified. This is automatically done through GET_DATA. In some cases, specify a phase interactively.

| Syntax | ENTER_PHASE |
|-------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Options | Description and Information |
| Phase name | <p>Name of phase: <Phase name></p> <p>The phase name is any string starting with a letter and containing only letters, digits or the underscore character. The phase name must be unique.</p> <p>Type code: <Phase-type code></p> <p>The Phase-type code must be specified for the phase if it is not an ordinary solution phase. Press <Enter> if the phase is ordinary.</p> |
| Phase-type | |
| G | <p>Gaseous mixture phase.</p>  <p>There may only exist one gas phase in a system.</p> |
| A | Aqueous solution phase. |
| L | Liquid solution phase but not A (aqueous) or Y (ionic liquid) |
| Y | Ionic liquid solution phase (that is specially treated by the Ionic Two Sublattice Liquid Model). |
| I | A phase with charged species but not G (gaseous), A (aqueous) or Y (ionic liquid). |
| F | An ordered FCC or HCP solution phase with four substitutional sublattices (additionally, such a phase can also have an interstitial sublattice). |
| B | An ordered BCC solution phase with four substitutional sublattices (additionally, such a phase can also have an interstitial sublattice). |
| Sublattice number | <p>Number of sublattices /1/: <Sublattice number></p> <p>Phases with stoichiometric constraints usually have two or more sublattices. On each sublattice one or more species can be entered as constituents. The number of sublattices must not exceed 10. Substitutional phases with no sublattices are treated as phases with one sublattice.</p> <p>Number of sites on sublattice # /1/: <Site number></p> <p>For phases with sublattices, the ratio of the sites on each sublattice (donated with #) must be given. The program asks for values for all sublattices (by repeating this question for each sublattice), but these may have a common factor extracted. It is recommended to use integer numbers as sites if possible. For substitutional phases with no sublattices, this question does not show up.</p> |
| Constituents | <p>Name of constituent: <Constituent name(s)></p> <p>For each sublattice specify at least one species as constituent. Several constituents can be</p> |

| Syntax | ENTER_PHASE |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>given consequently (on the repeated prompt) or on the same line separated by a space. This question is repeated till pressing <Enter> or giving a semi-colon (;), meaning that the list of constituents is terminated by (;) or an empty line.</p> <p>Will you add constituents later /N/:</p> <p>For Y add other constituents to the phase by specifying new components in e.g. an ENTER_PARAMETER command.</p> <p>If illegal constituents are used, you get a message e.g. when parameters are entered.</p> <p>Do you want a list of possible parameters /N/:</p> <p>Enter Y for a list of all possible parameters up to the fifth interaction order for the entered phase.</p> |


ENTER_SPECIES

Specify a species from the already entered elements. The stoichiometry of the species is the chemical formula of the species. For each species, its name and chemical formula must be given.



All elements are automatically entered simultaneously as species. The constituents of a phase must be species, but there is no thermochemical data associated with the species except as constituents of a phase.

| Syntax | ENTER_SPECIES |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>Species name: <Species name></p> <p>Enter a unique species name. This is usually its chemical formula but it can be any string which starts with a letter and contains only letters or digits. Parenthesis () and an underscore _ are permitted. The combination /- or /+ used to denote charge.</p> |
| Prompt | <p>SPECIES NAMES EXAMPLES</p> <p>NaCl2, Fe2O3, FeO3/2, Fe1O1.5, Ca.5Mg.5Si1O3,</p> <p>Al1H1O1_Al(OH) , Al1H1O1_HAlO, C2H4O3_124TRIOXOLANE, Na+, SiO4-4, H1/+1, H1O1/-1, AGC2N2-1.</p> <p>The species name can be used to separate isomers with the same stoichiometry, e.g. C2H2Cl2, (CHCl)2_cis, (CHCl)2_trans, CH2_CCl2.</p> |
| | <p>Stoichiometry /Species name/: <Chemical formula></p> <p>The elements in the chemical formula are normally separated by stoichiometric numbers. Neither parenthesis () nor an underscore _ is allowed in the chemical formula, while the special combination /- or /+ can be used.</p> |

| Syntax | ENTER_SPECIES |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>In upper case mode (see "REINITIATE" on page 242), the stoichiometric number unity can be excluded only if the element symbol consists of two letters. In lower case mode, the element must be typed with the first letter in UPPER case and the second in lower, and it is thus possible to distinguish CO (carbon monoxide) from Co (cobalt) without any stoichiometry number.</p> <div>  <p>All elements in a species must be entered prior to entering the species.</p> </div> |

ENTER_SYMBOL



This command is for the Gibbs Energy System (GES) module.



There are also a POLY and POST module commands with the same name. However, symbols entered in the GIBBS module are not the same symbols as defined in the POLY and POST modules.


In the GIBBS module, a symbol can be used to represent a numeric quantity (e.g. a *variable*), a *function*, or a *table*. The entered symbol (with a symbol name of maximum eight characters) can be used later when parameters are entered, and this is a flexible way to manipulate thermodynamic functions. Symbols are especially useful if the same function or table is used in several thermochemical parameters. A *parameter* symbol is used to assign the values of phase parameters (which are defined with the command ENTER_PARAMETER) to specific characterized symbols. If you want to define a constant quantity, enter it as a simple function with a constant value in all (temperature) ranges.

The symbols entered in the GIBBS module can also be listed and used in the PARROT module (for data optimization) where you can use the GIBBS-entered symbols (variables, functions or parameters) to define parameters that shall be optimized.



See [example 44](#) for an example of using variables and functions.

| Syntax | ENTER_SYMBOL |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>Variable, function, table or parameter? /Function/: <Keyword></p> <p>The keyword can be a variable, function, table or parameter.</p> |
| Prompt | <ul style="list-style-type: none"> Variables are similar to functions because these can also be expressions of state variables. It is possible to enter a variable with a new expression anytime. Functions are expressions of state variables or other functions. |

| Syntax | ENTER_SYMBOL |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <ul style="list-style-type: none"> • Tables are used for listing results. A table consists of a list of any number of state variables, functions or variables. • Parameter symbols are used to assign the values of phase parameters (which are defined by the command ENTER_PARAMETER) to specific characterized symbols. If the phase parameter is not defined yet, the parameter symbol is assigned zero or a symbol which is valued as zero. In this way it is easy to refer to entered phase parameters in further defining other phase parameters. <p>Name: <Name of the symbol></p> <p>Each symbol has a unique name that must start with a letter and can have maximum 8 characters.</p> <p>The following prompts are based on the type of symbol.</p> |
| Variable symbol | <p>Value: <Numeric value of a variable></p> <p>Only a constant numeric value, not an expression, is accepted.</p> |
| Function symbol | <p>Enter the lower-temperature limit, the expression, an upper-temperature limit and if there is another expression above this upper limit:</p> <p>Low temperature limit /298.15/: <Lowest temperature limit in K></p> <p>Specify the lowest-temperature limit, below which its (first) expression is not applicable. The default lowest limit of all kinds of data is 298.15 K.</p> <p>If a negative number is given as the lowest-temperature limit, it is assumed that there are breakpoints in pressure for this function; in such a case, it is interpreted as the lowest-pressure limit (in Pascal), and the other limits in the current function are also taken as pressure limit values (in Pascal).</p> <p>The temperature/pressure limits for the functions are checked during calculations. An indicator is set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit; and in such a case, an extrapolation is conducted using the TP-FUNCTIONS valid in the nearest temperature/pressure range.</p> <p>Function: <Definition for a TP-function></p> <p>A TP-Function consists of terms in T and P. The expression is a FORTRAN-like expression and operators +, -, *, = and ** can be used (** only with integer powers). Unary-functions LN or LOG (both for natural logarithm) and EXP (for exponential) can also be used. An expression can be continued on more than one line. A PT-function must be terminated by a semicolon (;) or an empty line. No more than 78 characters can be written on a line. If this is not sufficient space on one line, press <Enter> and continue on the next line. The program prompts with an ampersand & when a continuation is expected.</p> <div>  <p>A function can have several temperature ranges, and a different expression (i.e. a TP-Function) for each region; if required, a single function can have up to ten different temperature ranges (and thus have up to ten different TP-Functions).</p> </div> <p>This question is repeated if the current function has more than one expression (TPFunction) in various temperature ranges [or pressure ranges; only if the <i>lowest limit</i> is entered as a negative</p> |

| Syntax | ENTER_SYMBOL |
|--------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>number)).</p> <p>& <Continuation of the definition for the current TP-Function></p> <p>This is for a continuation of the definition for the current TP-Function. The ampersand & means that you can continue to write the function on the new line if one line is not enough for the current TP-Function. If you are finished the current TP-Function, press <Enter> again.</p> <p>High temperature limit /6000/: <High temperature limit in K></p> <p>For a TP-Function, specify the high-temperature limit, above which its current expression is not applicable. The default high-temperature limit for all kinds of data is always 6000 K.</p> <p>This question is repeated if the function has more than one expression (TPFunction) in various temperature ranges.</p> <div data-bbox="375 699 423 751"> </div> <p>All the temperature limits for the presently-be-entered TP-Function MUST be in an increasing order; otherwise the whole function is given a single value of zero.</p> <p>If a negative number is given as the lowest-temperature limit, it is interpreted as the low-pressure limit (in Pascal), and the high-temperature limit is also taken as the high-pressure limit (in Pascal) for the current TP-Function.</p> <p>The high-temperature/pressure limit for the current applicable expression (TPFunction) is the low temperature/pressure limit for the next range if several ranges are needed to describe the temperature/pressure-dependence of this function.</p> <p>The temperature/pressure limits for the functions are checked during calculations. An indicator is set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit; and in such a case, an extrapolation is conducted using the TP-Function valid in the nearest temperature/pressure range.</p> <p>Any more ranges /N/: <Y or N></p> <p>Answer N to finish the definition of the current function. If Y the program asks for a new function valid above the last high temperature limit and below a new high temperature limit. The maximum number of temperature ranges is 10.</p> <p>Important note: Make sure that the function and its first derivatives are continuous across break points.</p> |
| Table symbol | <p>Specify the low and high temperature limits, temperature step and tabled value at each specified temperature:</p> <p>Low temperature limit /298.15/: <Low temperature limit in K></p> <p>The lowest temperature where the table has a value.</p> <p>High temperature limit /6000/: <High temperature limit in K></p> <p>The highest temperature where the table has a value.</p> <p>Step in temperature /100/: <Temperature step></p> <p>The step in temperature between each value in the table. This step must be constant for the</p> |


| Syntax | ENTER_SYMBOL |
|------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>whole table. If a table cannot be described with a single step it must be divided into several tables for different temperature ranges. The upper and lower limits are truncated to give reasonable values where the table values must be specified.</p> <p>Table value at XX /YY/: <Table value></p> <p>The value of the table at the specified temperature (xx) must be given. The default value (yy) is the last value.</p> |
| Parameter symbol | <p>Input the correct name of a phase parameter (including its identifier, phase name, constituent and interacting constituent(s) in various sublattices (if exist), and degree of the parameter. Most of the settings are the same as in the "ENTER_PARAMETER" on page 223 command or the Function symbol prompts above.</p> <p>Parameter: <Parameter name></p> <p>Specify a correct and complete parameter name, which should contain all the necessary parts of the general form:</p> <p><Identifier>(<Phase>,<Constituent array>;<Digit>)</p> <p>If a parameter name is not acceptable or <Enter> is pressed, this error message displays:</p> <p>*** Error, please re-enter each part separately</p> <p>The program prompts for separate input for each required part for a parameter name.</p> <p>Identifier (/X/): <G or L, or TC, or BM, or V0 or VA or VC or VK></p> <p>Specify one of these types of legal identifiers.</p> <p>Phase name (/abcd/): <Phase name></p> <p>Specify the phase name.</p> <p>Constituent (in sublattice # /abc/): <Species name></p> <p>Specify the constituent name on the specified sublattice site of the given phase.</p> <p>Interacting constituent (in sublattice # /XYZ/): <Species name></p> <p>Specify the interacting constituent name on the specified sublattice site of the given phase; if there is no interacting constituent, press <Enter>.</p> <p>Interacting constituent (in sublattice # /XYZ/): <Species name></p> <p>If there is more than one interacting constituent on the specified sublattice site of the given phase, specify them; otherwise press <Enter>.</p> <p>Degree /#/ : <Degree></p> <p>Specify an integer number (a value from 0 through 9) as the degree for the phase parameter.</p> <p>Low temperature limit /298.15/: <Lowest temperature limit in K></p> <p>Specify the lowest-temperature limit (in Kelvin), or the lowest-pressure limit (in Pascal but entered as a negative number), for the current TP-Function.</p> <p>Function: <Definition for a function></p> |

| Syntax | ENTER_SYMBOL |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>Specify the desired TP-Function for the current temperature range (or current pressure range; only if the <i>lowest limit</i> is entered as a negative number).</p> <p>& <Continuation of the definition for the current TP-function></p> <p>Specify the desired TP-Function continuation for the current temperature range (or current pressure range; only if the lowest limit is entered as a negative number).</p> <p>High temperature limit /6000/: <High temperature limit in K></p> <p>Specify the high-temperature limit (in Kelvin), or the high-pressure limit (in Pascal; only if the lowest limit is entered as a negative number) for the current TP Function.</p> <p>Any more ranges /N/:</p> |

LIST_CONSTITUTION



This command is for the Gibbs Energy System (GES) module.

| Syntax | LIST_CONSTITUTION |
|------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------|
| | List all the constitutions (as site-fractions) for all the phases in the defined system. |
|  | This is mainly for software managers. There are no commands in the GIBBS monitor to set the constitution. |

LIST_DATA



This command is for the Gibbs Energy System (GES) module.

All data for the current system that is defined (retrieved from database in the DATA module, or directly entered in the GIBBS module) within the current GIBBS workspace is written in a readable manner on the output file. If no output file is specified, the data display on screen.

The output data consists of a list of all elements and their data followed by a list of all phases and the data associated with each phase. The thermochemical parameters listed for each phase are always in SI units.



For encrypted commercial databases you may not be able to use this command to list any retrieved data. However, it can be used to list some basic definitions (such as phase models and phase-constituents) retrieved from an encrypted database, as well as all the references related to original assessments (but not thermodynamic parameters) for the currently-defined system.

| Syntax | LIST_DATA |
|---------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Output to screen or file /Screen/: <File name></p> <p>Specify the name of a file in which the data shall be written in a readable manner. The default value is the screen (by pressing <Enter>).</p> |
| | <p>Options?: <Option(s)></p> <p>Choose one or several of these options for output:</p> <ul style="list-style-type: none"> • N the output is written as a user database format. • P the output is written as a macro file for future input. This is useful for creating *SETUP files for data assessments. • S the symbols are suppressed. • R the references for the parameters are listed (only for some databases in which references are available) • L the output is written suitable for a LaTeX preprocessor. |

LIST_PARAMETER



This command is for the Gibbs Energy System (GES) module.




There is also a PARROT module command with the same name.

List the TP-function(s) of a specific parameter for a phase. You must supply the name of the phase parameter:

The parameter name: <Identifier>(<Phase>,<Constituent array>;<Digit>)



For encrypted commercial databases, you may not be able to use this command to list any retrieved parameter.

| Syntax | LIST_PARAMETER |
|---------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Parameter: <Parameter name></p> <p>Specify a correct and complete parameter name, which should contain all the necessary parts of the general form: <identifier>(<phase>,<constituent array>;<digit>)</p> <p> See "About the ENTER_PARAMETER Command" on page 264 to learn how to define the parameter name.</p> <p>If a parameter name is not acceptable or <Enter> is pressed, an error message displays:</p> <pre>*** Error, please re-enter each part separately</pre> <p>The program prompts for separate input for each required part for a parameter name.</p> |

| Syntax | LIST_PARAMETER |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | Identifier (/X/): <G or L, or TC, or BM, or V0 or VA or VC or VK> Specify one of these types of legal identifiers. |
| | Phase name (/ABCD/): <Phase name> Specify the phase name. |
| | Constituent (in sublattice # /ABC/): <Species name> Specify the constituent name on the specified sublattice site of the given phase. |
| | Interacting constituent (in sublattice # /XYZ/): <Species name> Specify the interacting constituent name on the specified sublattice site of the given phase; if there is no interacting constituent, press <Enter>. |
| | Interacting constituent (in sublattice # /XYZ/): <Species name> If there is more than one interacting constituent on the specified sublattice site of the given phase, specify them; otherwise press <Enter>. |
| | Degree /#/ : <Degree> Specify a numerical number as the degree for the phase parameter. |

LIST_PHASE_DATA



This command is for the Gibbs Energy System (GES) module.

All data for a specific phase are written in a readable manner on screen. The thermochemical parameters listed for the phase are always in SI units.




For encrypted commercial databases you may not be able to use this command to list any phase data. However, this command can be used for listing some basic definitions (such as phase model and phase-constituents) for the specified phase, as well as all the references related to original assessments (but not thermodynamic parameters) for the currently-defined system.

| Syntax | LIST_PHASE_DATA |
|--------|-----------------------------------------------------------------------------------------|
| Prompt | Phase name: <Phase name> Specify a phase name (if abbreviated, it should be unique). |

LIST_STATUS



This command is for the Gibbs Energy System (GES) module.

| Syntax | LIST_STATUS |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>List the entered elements, phases and species with the status word. The command is included for system managers.</p> <div>  <p>Each element, species, phase and symbol has a set of status bits. The values of these bits are listed with this command.</p> </div> <p>The bits are listed as hexadecimal, i.e. four bits are written as a hexadecimal number. Two hexadecimal numbers make a byte. In hexadecimal, 0 to 9 mean normal digits. A to F means values 10 to 15. The number E4000000 has thus bit 1, 2, 3 and 6 equal to one. The bits are numbered starting with 1 for the most significant (leftmost) bit.</p> |

ELEMENT STATUS WORD

Set the element status word (*Bit. Meaning*) if:

1. Element cannot be deleted (only vacancy and electron)
2. Suspended (inclusive OR of bit 3 and 4)
3. Explicitly suspended
4. Implicitly suspended (cannot occur for an element)

SPECIES STATUS WORD

Set species status word (*Bit. Meaning*) if:

1. Species record for an element (each element has a species record)
2. Suspended (inclusive OR of bit 3 and 4)
3. Explicitly suspended
4. Implicitly suspended (e.g. if a species element is suspended)
5. Charged (inclusive OR of bit 6 and 7)
6. Negative charge
7. Positive charge
8. Vacancy
9. Component (by default the elements are the components)

PHASE STATUS WORD

Set phase status word (*Bit. Meaning*) if:

-
1. Ideal (no sublattices and no excess parameters)
 2. Suspended (inclusive OR of bit 3 and 4)
 3. Explicitly suspended
 4. Implicitly suspended (e.g. if all constituents suspended)
 5. Gas phase
 6. Liquid phase
 7. Solution phase
 8. Only one constituent (in each sublattice)
 9. Ions (inclusive OR of bit 10 and 12)
 10. New ionic liquid model (charge balance handled internally)
 11. Constituents cannot be added
 12. External charge balance needed
 13. Aqueous model
 14. Charged species (ions)
 15. Dilute entropy
 16. Last calculation exceeded temperature range for any parameter
 17. Kapoor-Frohberg-Gaye cell model
 18. Turbo calculation used
 19. Turbo calculation impossible
 20. Turbo calculation illegal
 21. Phase is not ideal
 22. Current site fractions saved
 23. This phase is the ordered part
 24. This phase is the disordered part (bit 2 and 3 also set)
 25. Shadow phase with diffusion data
 26. Error in ionic model
 27. Sometimes
 28. CVM-SRO (short-range ordering) entropy expression
 29. CVM initialization is made
 30. Used to test quasi-chemical ordering model
 31. Major constituents check even if no miscibility gap (ordering)

32. Hoch-Arpshofen model

SYMBOL STATUS WORD

Set symbol status word (*Bit meaning*) if:

1. Constant
2. Variable
3. Function
4. Table
5. Value must not be amended
6. Undefined

LIST_SYMBOL




This command is for the Gibbs Energy System (GES) module.

List the symbols available in the current GIBBS workspace, which are defined (retrieved from database in the DATA module, or directly entered in the GIBBS module) and used in TP-functions for the entered model parameters for various phases in the defined system.



For encrypted commercial databases you may not be able to use this command to list any retrieved symbol.

| Syntax | LIST_SYMBOL |
|---------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | Name: <Symbol name> Specify a symbol name (either as the full name of a defined symbol, or as the first few common characters of several symbols which have names starting with such common characters). |
| |  Only those symbols that match this name are listed. Or press <Enter> for a list of all the symbols defined (retrieved from database in the DATA module, or directly entered in the GIBBS module) for the current system, which are available in the current GIBBS workspace. |
| | Output to screen or file /Screen/: <File name> Specify the name of a simple-textual file in which the entered symbols shall be written in a readable manner (such a basic textual file can later on be opened and edited by any text editor). The default value is the screen (by pressing <Enter>). |

READ_GES_WORKSPACE




This command is for the Gibbs Energy System (GES) module.



This command or module is not available with GES6.

▶ ["Workspace Files" on page 26](#)

The data saved into a *.GES5 file with SAVE_GES_WORKSPACE can be read back into the GIBBS workspace.

| Syntax | READ_GES_WORKSPACE |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>Enter a File name and specify the working directory where to save the file in the Look in field. Normally the default file-type in the Files of type field is the correct one for the GES workspace format (i.e. *.GES5 file).</p> <div><p>The saved *.GES5 files are unique for each CPU type, and therefore a *.GES5 file saved on one CPU type cannot be read and used on another CPU type.</p></div> |


READ_WORKSPACES



This command is used in both the POLY and GES (GIBBS) modules.

▶ ["Workspace Files" on page 26](#)

The POLY3 and GIBBS workspaces and the calculated results from the MAP and STEP commands can be READ from a file where they are saved with SAVE_WORKSPACES. Such a *.POLY3 file is not printable.

| Syntax | READ_WORKSPACES |
|---------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>File name is the name of a saved POLY3-file where the POLY3 and GIBBS workspaces shall be read from must be specified. You do not need to type the extension if it is the default *.POLY3, otherwise type the whole POLY-file name.</p> |
| Options | <div><p>A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.</p></div> <p>A window opens so that the path (in the Look in field) and File name can be specified. The Files of type (i.e. POLY3) cannot be changed. Click Open to open the POLY3 and GIBBS workspaces from the saved *.POLY3 file.</p> |
| | <p>When reading back an original POLY3 workspace that has already been saved as an *.POLY3 file in the current Thermo-Calc (Console Mode) run or had been read from an existing POLY3 file under</p> |

| Syntax | READ_WORKSPACES |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | the current work area, while some additional changes in the settings may be made but do not need to be kept in further steps in the current Thermo-Calc (Console Mode) run or any diagram is plotted in the POST module, you can type <code>READ,,</code> or <code>READ_WORKSPACE ,,</code> |

RECOVER_START_VALUES


| Syntax | RECOVER_START_VALUES |
|--------|--------------------------------------------------------|
| | Recovers the start values in equilibrium calculations. |


REINITIATE



This command is for the Gibbs Energy System (GES) module.

All data in the stored GIBBS workspace are erased, and all variables are initiated to their default values.

| Syntax | REINITIATE |
|---------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Upper case only /Y/:</p> <p>Press <Enter> to keep the default where the name of elements and species is in only UPPER case. Or choose N to have the elements with two letter names with the first letter in Upper case and the second in lower case.</p> <div>  <p>In upper case mode all input in lower case is automatically converted to upper case.</p> </div> |
| | <p>Lower temperature limit /298.15/: <Lowest T in K></p> <p>This value is used as the lower temperature limit when data are entered interactively.</p> |
| | <p>Upper temperature limit /6000/: <Highest T in K></p> <p>This value is used as the upper temperature limit when data are entered interactively.</p> |
| | <p>Default element reference state symbol index /1/: <1 or 2 or 3></p> <p>Specify a proper index for the default listing parameters (symbol), or press <Enter> to accept the preset index 1.</p> <p>The <i>index</i> is for defining the symbol printed in listings of parameters. The symbol can be:</p> <ul style="list-style-type: none"> • G: the data are referred to Gibbs energy at a variable temperature (also called <i>Lattice Stability</i>). • H298: the data are referred to the enthalpy of the element at 298.15 K and 1 bar. • H0 is the same as H298 but at the temperature 0 K. |

| Syntax | REINITIATE |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| |  The index only changes the symbol, not any value. Normally the index is set correctly by the database. Only when manually entering data must you set the index to get the correct symbol. Set the index value to 0 to get the symbol G , to 1 to get the symbol H_{298} and to 2 to get H_0 . |

SAVE_GES_WORKSPACE




This command is for the Gibbs Energy System (GES) module.



This command or module is not available with GES6.

► ["Workspace Files" on page 26](#)

The data used by the GES workspace can be saved in a file (with a default extension GES5 under MS-Windows, or ges5 under Linux). The default file name is RESULT.GES5 or equal to the one used in a previous READ_GES_WORKSPACE command.

| Syntax | SAVE_GES_WORKSPACE |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>Enter a File name and specify the working directory where to save the file in the Save in field. Normally the default file-type in the Files of type field is the correct one for the GIBBS workspace format (i.e. *.GES5 file).</p>  The output is unformatted and cannot be printed. |

SAVE_WORKSPACES



This command is available for both the POLY and GES (GIBBS) modules.

► ["Workspace Files" on page 26](#)

You can save the current status and workspaces, including thermodynamic data, conditions, options and results from a single, stepping or mapping calculation on a *.POLY3 file. The workspaces are saved to a file with this command. This is useful so you have access to the workspace for later use or when you need to terminate the current Console Mode session.

- In the Gibbs (GES) module workspace, all thermochemical data are stored.
- In the POLY module workspace, all the last set of conditions and equilibrium state, changed status, entered symbols, advanced options, defined stepping/mapping

variables, added initial equilibria, stepped/mapped results, etc., are stored, so it also contain the GES workspace.

- When you are in a response-driven module such as POTENTIAL or SCHEIL for example, a workspace file is automatically opened. In the workspace file, system definitions, conditions for the calculation, calculation results, and plot settings are saved. The file is saved in the current working directory, and is named after the name of the module that created it. For example, the POTENTIAL module saves a workspace file called `POT.POLY3` ; the POURBAIX module saves a file called `POURBAIX.POLY3` and so forth.



After a `SAVE_WORKSPACES` command, you can always come back to exactly the state you had when you issued the command by giving a `READ_WORKSPACE` command. For example, after saving the POLY and GIBBS workspaces to a file, you can leave the program and at a later time `READ` the file and continue from the saved state.


IMPORTANT INFORMATION ABOUT MAP AND STEP COMMANDS




A `STEP` or `MAP` command automatically saves the workspace with the most recently specified name. Do not use the `SAVE_WORKSPACES` command after a `MAP` or `STEP` command.

The results from the `STEP` or `MAP` commands are destroyed by the `SAVE_WORKSPACE` command. You can append several results obtained by sequential `STEP` or `MAP` calculations without destroying the previous results, whilst `SAVE_WORKSPACE` erases them all. Keeping this in mind is important and useful particularly for calculating various isothermal (or isoplethal) sections and plotting them on the same diagram in a single Thermo-Calc run.

To suspend some of the `STEP` or `MAP` results, use the `AMEND_STORED_EQUILIBRIA` command.

| Syntax | SAVE_WORKSPACES |
|---------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | A <code>file name</code> must be specified. The default extension of the POLY workspace file is <code>*.POLY3</code> but you can have any other file extension. |
| Options |  Linux and Mac are case sensitive so ensure you enter <code>.POLY3</code> . A Save window displays if a file name is not given after the command, so that the path (in the Save in field) and File name can be specified. The Files of type cannot be changed. |

| Syntax | SAVE_WORKSPACES |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>If there is already a file with the same file name under the directory a warning message displays. Click OK to overwrite the current POLY or GIBBS workspace onto the existing file. Click Cancel to return to the module. You can use the SAVE command with an unspecified name (i.e. through <code>SAVE , , ,</code> command-sequence) to save the POLY or GIBBS workspace.</p> <div>  <p>When saving a POLY3 workspace under a name that already exists under the current work area, which is saved by default (after running a special module, e.g. BIN, TERN, POT, SCHEIL and POURBAIX) or in an earlier stage of the current Console Mode session or in a previous run (which is READ into the current POLY3 workspace), you can type <code>SAVE, , Y</code> or <code>SAVE_WORKSPACE , , Y</code>. However, this must also be avoided if some results from previous MAP or STEP calculations shall not be destroyed.</p> </div> |

SET_R_AND_P_NORM

The value of the gas constant (R) is used to define the energy units that are used for input of data. On output, all data are in SI units. The value of the pressure 1 atm is used to interpret values of the pressure given by application programs.

| Syntax | SET_R_AND_P_NORM |
|---------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Value of gas constant in your energy units /8.31451/: <New value></p> <p>The default value of the gas constant is in SI units (i.e. 8.31451). If you change this value, it only affects the interpretation of energy data given interactively from the terminal, e.g. if the value is set to 1.98717 you can give values in Calories.</p> |
| | <p>Value of one bar in your pressure units /100000/: <New value></p> <p>The value of the pressure given in application programs is divided by this value and then multiplied with the value of one bar expressed in Pascal before it is used inside the GIBBS module.</p> |

SCHEIL Module Commands

In this section:

| | |
|------------------------------------|-----|
| BCC_TO_FCC_TRANSFORMATION | 247 |
| EVALUATE_SEGREGATION_PROFILE | 247 |
| GLOBAL_MINIMIZATION | 248 |
| LIQUID_PHASE_NAME | 248 |
| SAVE_FILE_NAME | 248 |
| SET_NUMERICAL_LIMITS | 249 |
| START_WIZARD | 250 |
| TEMPERATURE_STEP | 253 |
| TERMINATION_CRITERIA | 253 |
| USE_BACK_DIFFUSION | 253 |

BCC_TO_FCC_TRANSFORMATION



This command is for the SCHEIL module.

Use this command to allow transformations in the solidified part of the alloy caused by each of the components specified to be fast diffuser.



It is recommended that you only select this for steels.

| | |
|--------|------------------------------------------------------------|
| Syntax | BCC_TO_FCC_TRANSFORMATION |
| Prompt | Allow bcc → fcc ? /N/ Enter Y to allow transformations. |


EVALUATE_SEGREGATION_PROFILE



This command is for the SCHEIL module.

Use this command in order to evaluate a segregation profile while performing the Scheil calculation. The Scheil calculation itself does not contain a spatial dimension. However, if it is assumed that the molar volume is constant and equal for all elements, and if a length is provided over which solidification occurs (for example the secondary dendrite arm spacing) then the generated profile corresponds to the segregation that would be obtained under the assumptions of a Scheil calculation. The grid is then equidistant and can be used as input for a DICTRASimulation.

The generated text file contains, on each line, the mole fractions of all elements in alphabetical order at a certain grid point. If the composition is the same on several consecutive lines it means that the composition of the then remaining liquid has reached a state in which there are no degrees of freedom.

| | |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | EVALUATE_SEGREGATION_PROFILE |
| Prompt | Evaluate segregation profile? /N/  If the answer is Y, a segregation profile will be evaluated and saved to disc. Note that this feature is not supported with back diffusion; if back diffusion is enabled no segregation profile will be generated. |
| | Number of grid points /100/ Enter the number of grid points for the segregation profile. A file dialogue window opens and allows you to specify the name of the file in which the segregation profile is written. |

| Syntax | EVALUATE_SEGREGATION_PROFILE |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | In a macro file it is possible to enter all arguments on a single line, e.g. <code>EVALUATE_SEGREGATION_PROFILE Y 100 XF.TXT</code> , meaning that the segregation profile is evaluated over 100 grid points and saved to a file (XF.TXT) in the current working directory. |

GLOBAL_MINIMIZATION



This command is for the SCHEIL module.



["ADVANCED_OPTIONS" on page 135](#) for information about that GLOBAL_MINIMIZATION command.

| Syntax | GLOBAL_MINIMIZATION |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | Use global minimization? /N/ |
| Prompt | The default (N) does not use global minimization. If you choose Y, the global minimization is done when possible (depending on the conditions setting), and a global minimization test is performed when an equilibrium is reached. This costs more computer time but the calculations are more robust. |

LIQUID_PHASE_NAME



This command is for the SCHEIL module.

Use this command to use the liquid phase name from the database definitions or enter another phase name.

| Syntax | LIQUID_PHASE_NAME |
|--------|-----------------------------------------------------------------------------------------------|
| | Liquid phase name /Default/ |
| Prompt | Default selects the liquid phase from the database definitions, otherwise enter a phase name. |


SAVE_FILE_NAME



This command is for the SCHEIL module.

Use this command to save the file. The files get the console number added to this name, e.g. `005.->Scheil_006.POLY3` and `Scheil_segregation_profile.txt`).

| Syntax | SAVE_FILE_NAME |
|--------|-----------------------------------------------------------|
| Prompt | Name of files to be saved, POLY and segregation profiles. |

| | |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | SAVE_FILE_NAME |
| |  Linux and Mac are case sensitive so ensure you enter .POLY3. |

SET_NUMERICAL_LIMITS



This command is available for the POLY, Scheil and ED-EXP modules.


Change the criteria for convergence. This is to speed up a calculation in a complex system.

If there is any convergence problem in finding a stable solution at any stage during a calculation procedure enforced by COMPUTE_EQUILIBRIUM, STEP_WITH_OPTIONS, MAP or ADVANCED_OPTIONS), this message displays:

```
Convergence problems, increasing smallest site-fraction from
1.00E-30 to hardware precision 2.00E-14. You can restore using
SET-NUMERICAL-LIMITS
```

This implies that smallest site fraction in the current POLY workspace is automatically increased from the default value 1.00E-30 to the hardware-dependent precision (under Linux, as 2.00E-14). For other subsequent POLY module calculations, you can use this command to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

| | |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | SET_NUMERICAL_LIMITS |
| Prompt | <p>Maximum number of iterations /500/:</p> <p>By default, the program tries 500 iterations before it gives up. As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.</p> |
| | <p>Required accuracy /1E-6/:</p> <p>This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.</p> |
| | <p>Smallest fraction /1E-12/:</p> <p>This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions.</p> <p>The default value for the smallest site-fractions is 1E-12 for all phases, except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as 1E-30 (unless you have used the SET_NUMERICAL_LIMITS command to reset an even-lower value (e.g. 1E-45, that is naturally enforced to all the phases in the system).</p> |
| | <p>Approximate driving force calculation for metastable phases /Y/:</p> <p>Normally the POLY module only requires that the set of stable phases is in equilibrium in order to</p> |

| Syntax | SET_NUMERICAL_LIMITS |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>terminate the iterations. By default, the metastable phases are included in all iterations but these may not have reached their most favourable composition and thus their driving forces may be only approximate.</p> <p> If it is important that these driving forces are correct, choose N to force the calculation to converge for the metastable phases. This may require more iterations, and the STEP and MAP command may also terminate due to bad convergence in a metastable phase.</p> |

START_WIZARD



This command is for the SCHEIL module.



["About the Scheil-Gulliver Solidification Simulations " on page 72](#)

Use this command to use the START_WIZARD with step-by-step prompts to create a basic Scheil simulation.


You are prompted for settings including the major element or alloy, composition input in mass (weight) percent, the alloying elements, the temperature, fast diffusing components, and whether any phase should have a miscibility gap check. If back diffusion is enabled using the USE BACK DIFFUSION command, there are additional prompts included in the Start Wizard and described below.




The Scheil with back diffusion feature is only available for systems with diffusion data, i.e. it requires the use of a mobility database.

Use the other commands to make changes to settings that are not included in this wizard.

- BCC_TO_FCC_TRANSFORMATION
- EVALUATE_SEGREGATION_PROFILE
- GLOBAL_MINIMIZATION
- LIQUID_PHASE_NAME
- SAVE_FILE_NAME
- STORED_COMPOSITION_TYPE
- TEMPERATURE_STEP
- TERMINATION_CRITERIA

| Syntax | START_WIZARD |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>The following is a list of the prompts. Press <Enter> to accept the defaults that are shown between the forward slashes (/default/).</p> <p>Database /<Default>/:</p> <p>The available thermodynamic database and its version are available to enter (based on license). Enter ? for a list.</p> <p>Major element or alloy:</p> <p>The major element in the system, e.g. Fe for a steel.</p> <p>Composition input in mass (weight) percent? /Y/:</p> <p>Set whether to specify the Composition input in mass (weight) percent (the default) or in Mole percent. Enter Y for mass percent and N for mole percent.</p> <p>1st alloying element:</p> <div style="border: 1px solid black; padding: 10px; margin: 10px 0;">  You can specify all the alloying elements and their corresponding compositions on the same line when you are prompted to specify your first alloying element. For example, you can enter Cr 5 Ni 1 Mo 0.5 C 0.01 N 0.02. </div> <p>You can directly specify mass or mole percent after the name (for example, enter Cr 5). If this is not specified, then you are prompted to enter it separately.</p> <p>Mass (weight) percent /1/</p> <p>2nd alloying element:</p> <p>Specify the other alloying elements in the same way as you specify the first (for example, c 1).</p> <p>Mass (weight) percent /1/</p> <p>Next alloying element:</p> <p>After you have specified your last alloying element, press <Enter> when requested to specify the next element. This ends the process of defining the bulk composition of the alloy system.</p> <p>Temperature (C) /2000/:</p> <p>Enter a value for the temperature in degrees C (Celsius) . This value should be sufficiently high so that the solidification simulation starts with the alloy system in the liquid single-phase region.</p> <p>Decide which phases (if any) to reject at the Reject phase(s) prompt. Enter the name of the phases to reject or press <Enter> for NONE.</p> <p>Decide whether to Restore phase(s). You may want to restore a phase that you rejected when you ran the simulation earlier, or you may want to restore a phase that is rejected by default in your database. Enter the name of the phases to restore or press <Enter> for NONE.</p> <p>Then you are asked to confirm whether these phases should be retained in this system:</p> <p>OK? /Y/:</p> <p>Press <Enter> to accept the default Y or type N and press <Enter>. Thermodynamic data about the</p> |

| Syntax | START_WIZARD |
|-------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>alloy system you defined is retrieved from the database.</p> <p>Should any phase have a miscibility gap check? /N/:</p> <p>If you answer <code>Y</code>, you are prompted to specify the Phase with miscibility gap. Answer with a solution phase name(s) (e.g. <code>FCC</code>) as well as the Major constituents for sublattice (for each sublattice site) (for this example, <code>Cr</code> is entered for sublattice 1 and <code>C</code> for sublattice 2).</p> <p>Press Enter to specify another phase.</p> <p>Fast diffusing components: /None/:</p> <p>Enter the elements that diffuse fast in solid phases and can assume to be in equilibrium in the whole phase. E.g. C in a steel.</p> |
| Back Diffusion settings | <p>If the "USE_BACK_DIFFUSION" on the next page command is set to <code>Y</code> to enable back diffusion, the following prompts are included with the Start Wizard at various points in the set up:</p> <p>Mobility Database /<Default>/:</p> <p>The available mobility database and its version are available to enter (based on license). Enter ? for a list.</p> <p>You then are shown a list of what phases are available for the database and the defined system and have the opportunity to reject or restore phases at the next prompts.</p> <p>Reject phase(s) /NONE/:</p> <p>Restore phase(s): /NONE/:</p> <p>Then you are asked to confirm whether these phases should be retained in this system:</p> <p>OK? /Y/:</p> <p>Press <Enter> to accept the default <code>Y</code> or type <code>N</code> and press <Enter>.</p> <p>Temperature time dependence /LINEAR/:</p> <p>Specify the type of temperature time dependence. Press <Enter> to accept this default.</p> <p>An increased value moves the result from equilibrium toward a Scheil-Gulliver calculation.</p> <div>  <p>LINEAR is currently the only available option and it corresponds to a constant cooling rate.</p> </div> <p>Cooling rate (K/s) /.1/:</p> <p>Specify the cooling rate in Kelvin per second (K/s). An increased value moves the result from equilibrium toward a Scheil-Gulliver calculation.</p> <p>Expression for secondary dendrite arm spacing /CONSTANT/:</p> <p>Secondary dendrite arm spacing is the distance in meters (m) between two secondary dendrite arms. Specify the type of secondary dendrite arm spacing by entering <code>CONSTANT</code> (the default) or <code>POWER_LAW</code>.</p> <p>An increased value moves the result from equilibrium toward a Scheil-Gulliver calculation. Use</p> |

| Syntax | START_WIZARD |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <ul style="list-style-type: none"> • CONSTANT for a constant dendrite arm spacing. If you choose this, then enter a value for the Secondary dendrite arm spacing (m) /5E-05/: prompt. • POWER_LAW in the form $c * (\text{cooling rate})^n$ where <i>c</i> and <i>n</i> are entered in the next prompts. If you choose this, then enter a value for the Exponent <i>n</i> /.33/: and Scaling factor <i>c</i> /5E-05/: <p>Primary phase /AUTOMATIC/:</p> <p>Specify the phase name or <i>Automatic</i> (default) for the primary phase. The primary phase is the phase where the back diffusion takes place. If <i>Automatic</i> is selected, the program tries to find the phase which will give the most back diffusion. That behavior can be overridden by selecting a specific primary phase.</p> |

TEMPERATURE_STEP



This command is for the SCHEIL module.

Use this command to define a temperature step.

| Syntax | TEMPERATURE_STEP |
|--------|------------------------------|
| Prompt | Set temperature step (C) /1/ |

TERMINATION_CRITERIA



This command is for the SCHEIL module.

Use this command to define the termination criteria for the fraction of liquid or temperature.

| Syntax | TERMINATION_CRITERIA |
|---------|-------------------------------------------------|
| Prompts | Fraction of liquid or Temperature (F or T)? /F/ |
| | Fraction of liquid /.01/ |

USE_BACK_DIFFUSION



This command is for the SCHEIL module.



The Scheil with back diffusion feature is only available for systems with diffusion data, i.e. it requires the use of a mobility database.

▶ ["About the Scheil-Gulliver Solidification Simulations " on page 72](#)

The USE_BACK_DIFFUSION command enables back diffusion in the solid primary phase. Once enabled, there are additional prompts and settings that are included and described with the ["START_WIZARD" on page 250](#) command.

| | |
|--------|-----------------------------------------------------------------------------------------------------------------------|
| Syntax | USE_BACK_DIFFUSION |
| Prompt | Use back diffusion? /N/ The default (N) does not use back diffusion. If you choose Y, then back diffusion is used. |

PARROT Module Commands

► ["The PARROT Module" on page 9](#) in the *Data Optimization User Guide*.

In this section:

| | |
|-----------------------------------------|-----|
| AMEND_PARAMETER | 257 |
| AMEND_SYMBOL | 259 |
| COMPILE_EXPERIMENTS | 261 |
| CONTINUE_OPTIMIZATION | 262 |
| CREATE_NEW_STORE_FILE | 263 |
| EDIT_EXPERIMENTS | 263 |
| About the ENTER_PARAMETER Command | 264 |
| LIST_ALL_VARIABLES | 270 |
| LIST_CONDITIONS | 270 |
| LIST_PARAMETER | 271 |
| LIST_PHASE_DATA | 272 |
| LIST_RESULT | 272 |
| LIST_STORE_FILE | 276 |
| LIST_SYMBOL_IN_GES | 276 |
| OPTIMIZE_VARIABLES | 277 |
| READ_PARROT_WORKSPACES | 277 |
| RECOVER_VARIABLES | 278 |
| REINITIATE | 278 |
| RESCALE_VARIABLES | 278 |
| SAVE_PARROT_WORKSPACES | 278 |
| SET_ALTERNATE_MODE | 279 |
| SET_EXTERNAL_PARAMETER | 279 |
| SET_FIX_VARIABLE | 280 |

| | |
|--------------------------------|-----|
| SET_OPTIMIZING_CONDITION | 281 |
| SET_OPTIMIZING_VARIABLE | 282 |
| SET_OUTPUT_LEVELS | 283 |
| SET_SCALED_VARIABLE | 283 |
| SET_STORE_FILE | 284 |

AMEND_PARAMETER




This command is for the PARROT module.




There is also a Gibbs (GES) module command with the same name.

Interactively modify the TP-function(s) for a specific parameter for a phase with this command. This is useful in order to correct typing errors because the old function is made available for interactive editing on the terminal.

| Syntax | AMEND_PARAMETER |
|---------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Parameter: <Parameter name></p> <p>Specify a correct parameter name. If a parameter name is not acceptable or <Enter> is pressed, the error message displays:</p> <p>*** Error, please re-enter each part separately</p> <p>The program prompts for separate input for each part for a parameter name.</p> |
| | <p>Identifier (/X/): <G or L, or TC, or BM, or V0 or VA or VC or VK></p> <p>Specify one of these types of legal identifiers</p> <p> "ENTER_PARAMETER" on page 268</p> |
| | <p>Phase name (ABCD/): <Phase name></p> <p>Specify the phase name.</p> |
| | <p>Constituent (in sublattice # /ABC/): <Species name></p> <p>Specify the constituent name.</p> |
| | <p>Interacting constituent (In sublattice # /XYZ/): <Species name></p> <p>Specify the interacting constituent name; if there is no interacting constituent, press <Enter>.</p> |
| | <p>Interacting constituent (in sublattice # /XYZ/): <Species name></p> <p>If there is more than one interacting constituent, specify these; otherwise press <Enter>.</p> |
| | <p>Degree /#/ : <Degree></p> <p>Specify a numerical number as the degree of the phase parameter.</p> |
| | <p>After the parameter name is specified correctly, the program lists its current definition (either preset in database or defined by the ENTER_PARAMETER command), such as:</p> <pre>L (PHASE2,AL,MG;1)= 298.15<T<2000.00: +5000 2000.00<T<4500.00: +4500 4500.00<T<6000.00: +4000</pre> |

| Syntax | AMEND_PARAMETER |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>You are prompted to change the parameter definition:</p> <p>Do you want to change the number of ranges /No/:</p> <p>Enter Y to change the number of ranges for the chosen function, or change some of the temperature limits in the definition, then retype both the low/high temperature limits and functions</p> <p>If you do not want to change the number of ranges but want to change the function(s) in one or more ranges, press <Enter> and the whole definition of the chosen parameter in all ranges (if any) is listed such as:</p> <pre> DIFFERENT FUNCTIONS IN THESE RANGES 298.15<T<2000.00 2000.00<T<4500.00 4500.00<T<6000.00 </pre> <p>This message prompts:</p> <p>Do you want to change range limits /No/:</p> <p>If there is more than one range, this question is prompted. Press <Enter>.</p> |
| | <p>Range number (0 to exit) /0/: <Range number></p> <p>If the function of a parameter is different in two or more temperature ranges, you must specify the range of the function of which you want to amend. Or press <Enter> or type 0 to exit this command without making any change.</p> |
| | <p>Function</p> <p>The previous function is available for editing. The editing is performed within the general subroutine <code>FOOLED</code>, as described in "AMEND_SYMBOL" on the next page. This routine prompts as follows:</p> <pre>1:+:></pre> <p>The prompt consists of the current position in the string and the character at that position between colons, (::).</p> <h3>COMMANDS</h3> <p>These commands can be given:</p> <ul style="list-style-type: none"> • Help: ? • Move CP to last or first character: <+/-> A • Delete characters from CP: <+--#characters> D • Exit: E • Find: <#occurrences> F<string>@ • Insert: I<string>@ • Move: <+--#positions> M • Restore string: R |

| Syntax | AMEND_PARAMETER |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <ul style="list-style-type: none"> • Substitute: S<OLD>@<NEW>@ • Type string: T <p>Where CP denotes the current position in a string, # means number of, @ is a terminator of an input or search string.</p> <p> When the string is typed the character at the current position is replaced by an underscore _.</p> <p>To finish the editing of the current function, type E at the prompt.</p> |
| | <p>Range number (0 to exit) /0/: <Range number></p> <p>Give a range number to edit that function, or press <Enter> or type 0 to exit this command.</p> |

AMEND_SYMBOL



This command is for the PARROT module.



The same command is also available for the Gibbs (GES) module.

Interactively calculate the current values of a function or table (predefined by the switched database or previously entered with ENTER_SYMBOL) at the current temperature and pressure condition, and also possible to modify the definitions of variables or functions.




The current values of the temperature and pressure used to calculate the functions or tables are the ones listed with LIST_STATUS. There is no way to change the current temperature and pressure values interactively.

To modify the definitions of entered symbols (variable, functions or parameters), the performance of this command is slightly different one from another, as described below:

- For variables, the values can be changed.
- For functions the low and high temperature limits in various ranges (if any), as well the expressions, can be changed.
- For parameters the low and high temperature limits in various ranges (if any), as well the expressions, can be changed.

| Syntax | AMEND_SYMBOL |
|---------|--------------------------------------------------------------------------------|
| Prompts | <p>Name: <Symbol name></p> <p>Specify the name of an entered symbol.</p> |

| Syntax | AMEND_SYMBOL |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>For tables and functions (or parameters which are treated as functions after these are entered by the ENTER_SYMBOL command with the <code>Parameter</code> keyword, but not by the ENTER_PARAMETER command), after the symbol name is specified here, the program automatically calculates the values under the current temperature and pressure conditions, and lists the current values, such as:</p> <pre> FUNCTION VALUE 2.52500000E+01 TABLE VALUE 1.56000000E+02 </pre> <p>For variables and functions (or parameters), there are additional prompts and depend on the symbol type.</p> |
| | <p>For a variable, its current value is displayed, and you can change it to a new value:</p> <pre>Value /Current value/: <New value></pre> <p>For a function (or a parameter entered as a symbol):</p> <pre>Do you want to change the number of ranges /No/:</pre> <p>Enter Y to change the number of ranges for the function, or change some of the temperature limits in the definition, then retype both the low/high temperature limits and functions (see all the remaining details in the ENTER_SYMBOL command.</p> <p>If you do not want to change it, press <Enter>. The definition of the chosen function in all ranges (if any) is listed, for example:</p> <pre> DIFFERENT FUNCTIONS IN THESE RANGES 298.15<T<2000.00 2000.00<T<4500.00 4500.00<T<6000.00 </pre> <p>and this message displays:</p> <pre>Do you want to change range limits /No/:</pre> <p>If a function is different in two or more temperature ranges, you must specify the range of the function of which you want to amend. Or press <Enter> or type 0 to exit this command without making any change.</p> |
| | <pre>Range number (0 to exit) /0/: <Range number></pre> <p>Function:</p> <p>The previous function is available for editing. The editing is performed within the general subroutine FOOLED. This routine prompts as follows:</p> <pre>1:+:></pre> <p>The prompt consists of the current position in the string and the character at that position between colons (:).</p> <h2>COMMANDS</h2> <p>These commands can be given:</p> |

| Syntax | AMEND_SYMBOL |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <ul style="list-style-type: none"> • Help: ? • Move CP to last or first character: <+/-> A • Delete characters from CP: <+-#characters> D • Exit: E • Find: <#occurrences> F<string>@ • Insert: I<string>@ • Move: <+-#positions> M • Restore string: R • Substitute: S<OLD>@<NEW>@ • Type string: T <p>Where CP denotes the current position in a string, # means number of, @ is a terminator of an input or search string.</p> <div>  <p>When the string is typed the character at the current position is replaced by an underscore _.</p> </div> <p>To finish the editing of the current function, type E at the prompt.</p> |

COMPILE_EXPERIMENTS

The descriptions of the experimental equilibria saved on a textual *.POP file, given as commands in the POLY and ED_EXP syntax, is compiled by this command into the PARROT structured data, i.e. stored into the current work *.PAR file which is created with ["CREATE_NEW_STORE_FILE" on page 263](#), set by ["SET_STORE_FILE" on page 284](#), or opened with ["READ_PARROT_WORKSPACES" on page 277](#), all done before COMPILE_EXPERIMENTS.

This command also lists the compilation details on screen or onto a listing file (*.TXT).



If a syntax error in the commands is detected, the compilation is terminated. You need to correct the error in the *.POP file (using a textual editor) and recompile it with the *.PAR work (store) file.

After a successful compilation, the program translates all the experimental data points in the *.POP file into a graphical experimental data file (*.EXP) in the DATAPLOT syntax, which can be further edited and used as a graphical experimental data file (*.EXP) for the purposes of imposing onto calculated/plotted phase diagrams and/or property diagrams for comparisons during the assessment process.



DATAPLOT User Guide included with this documentation set.

| Syntax | COMPILE_EXPERIMENTS |
|---------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | A window displays to open the original experimental data file (*.POP). Enter a *.POP File name box, and specify the working directory in the Look in box. Normally the default file-type in the Files of type field is the correct one for the experimental data format (i.e. *.POP file). Click Open or Cancel button as applicable. |
| Prompts | <p>Output to screen or file /Screen/: <*.pop file name></p> <p>A list of the source code in the *.POP file and error messages during compilation is written on screen (by pressing <Enter>) or on a list *.TXT file under a specific file name which can later on be opened and edited by any basic textual editor.</p> |
| | <p>Initiate store file /Y/:</p> <p>After a successful compilation, the data in the POLY workspace is stored as a new block of equilibria on the current work (store) file. By default the store file is initiated before compilation and only the compiled block is stored on the current work file (consequently, the *.PAR file is updated).</p> <p>A window displays to generate/store the graphical experimental data file (*.EXP) in the DATAPLOT syntax. Enter a *.EXP file name in the File name field and specify the working directory when opening the *.EXP file in the Look in field. Normally the default file type in the Files of type field is the correct one for the graphical experimental data format (i.e. *.EXP file). Click Open or Cancel as applicable.</p> <p>To keep the current work file, enter N.</p> |

CONTINUE_OPTIMIZATION



This command is for the PARROT module.

This command continues the optimization using the same Hessian matrix.



In some cases it is not possible to attempt continuation. For example, if the optimization has already converged or if the optimizing parameters or the set of experimental equilibria used in the current optimization runs are changed. The program gives a warning message if you try to continue when you make these changes.

| Syntax | CONTINUE_OPTIMIZATION |
|---------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | Are you sure? /N/: <N or Y> |
| Prompts | <p>Prior to this question, a message displays to confirm if it is OK to continue:</p> <p>It is safe to CONTINUE only after TOO MANY ITERATIONS and no change in variables and experiments ...</p> <p>You can accept the default (N) in order to cancel this special attempt.</p> |
| | Number of iterations /N/: <Integral number of iteration> |

| | |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | CONTINUE_OPTIMIZATION |
| | Specify an integral number for the optimization iteration. The specified iteration number is shown as the default number. The PARROT program tries this exact number of different sets of values of the optimizing variables without stopping the optimization even it would have converged earlier or should give up earlier. |

CREATE_NEW_STORE_FILE



This file is hardware dependent and cannot be read by any text editor.

Create a binary file to be used as a *work file* (also called *store file*) before any optimization can be done. The workspace used by the GIBBS, POLY and PARROT modules is stored automatically on the work file but not any experimental information. The binary work file has a default extension of `PAR` under MS-Windows or `par` under Linux/UNIX.

A work file that is created at a previous run can be used in the PARROT module with the other command SET-STORE-FILE.

| | |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | CREATE_NEW_STORE_FILE |
| | <*.par file name> |
| Prompt | A Save window displays. Enter a File name and specify the working directory in the Save in field. Normally the default file-type in the Files of type field is the correct one for the PARROT workspace format (i.e. PAR file). Click Save or Cancel as applicable. |

EDIT_EXPERIMENTS

Initialize and make available the sub-module for editing experimental equilibria, i.e. the ED_EXP module. All experimental equilibria compiled from the *.POP file can be accessed in the ED_EXP module.

The ED_EXP module is similar to the normal POLY module, but some commands are special and some POLY commands are not available. In the ED_EXP module, you can calculate each equilibrium separately or together, provide start values for equilibria which failed to converge, set weights, and modify the values of experiments or conditions.

| | |
|--------|-----------------------------------------------------------------|
| Syntax | EDIT_EXPERIMENTS |
| | You are now in this submodule and can start using the commands. |

- The first required command after entering the ED_EXP module for the first time (from the PARROT module GOTO MODULE ED-EXP) should always be READ_BLOCK in order to load the experimental data block from the current work *PAR-file for

editing.

- The READ_BLOCK command must also be used prior to any other ED_EXP command if the module is reinitiated, or if no experimental data block is not previously read from a work file compiled with a proper experimental data .POP file, or if you want to change to another data block for editing.
- If any change is made in the ED_EXP module remember to use the command SAVE_WORKSPACE before going BACK to the PARROT module.



Although the TABLE_HEAD, COMMENT and FLUSH_BUFFER commands are visible in the ED_EXP module, these cannot be used here as these only work in a *.POP file (or *.DOP file for DICTRA).

About the ENTER_PARAMETER Command



For the PARROT Module, this command is the same and is described here. See ["ENTER_PARAMETER" on page 268](#) for the command details.

In the descriptions of the standard thermochemical properties and special physical properties for a phase, there are a number of parameters which may depend on the temperature and pressure. The expressions for these parameters can be given in a free form as a sum of terms with powers of T and P and may also include the natural logarithm and exponential function. This type of expression is called *TP-functions*. Identical parameters (in terms of parameter-names) are stored only once in the GIBBS workspaces.

The composition-dependence of the Gibbs energy is described in the GIBBS module by the internal data structure, which is created when the phase is entered (see ["Gibbs Energy System \(GES\) Commands" on page 202](#)). The Gibbs energy of a phase is always referred to one formula unit of the phase, i.e. the amount derived from the number of sites (i.e. the stoichiometric coefficient) for each sublattice. If vacancy is a constituent of a sublattice, the amount of matter per formula unit of the phase may vary with composition.

Defining the Parameter

A valid parameter should have the general form of:

```
<identifier>(<phase>, <constituent array>; <digit>) <xxx> <expression> <yyy>  
<keyword Y or N> <zzz> !
```

The identifier must be followed by an opening parenthesis, a phase name, a comma and a constituent array. Optionally, the constituent array can be followed by a semicolon and a digit. The parameter name is terminated by a closing parenthesis. The parameter form is defined as:

- `<identifier>` is the parameter type;
- `<phase>` is the phase name (maximum 24 characters);
- `<constituent array>` is the specific constituent array in the phase;
- `<digit>` is the degree of composition-dependent interaction contribution (an integer number from 0 through 9), that is only for excess energy (L), Curie temperature (TC) and Bohr magneton number (BMAGN), as well as for volume-related parameters (V0 or VA or VC or VK); if it is valued as zero, or if it is for the standard Gibbs energy (G) for which the degree is always zero, it can be omitted;
- `<expression>` is the mathematical relation to describe the parameter;
- `<xxx>` and `<yyy>` are the low and high temperature limits respectively for the applicable temperature range of the parameter expression;
- `<keyword Y or N>` is the indicator on if there is continuation for the parameter expression or not;
- `<zzz>` is the reference index/number for the assessment of this parameter;
- The exclamation point `!` is used to indicate that the current parameter definition is ended.

PARAMETER NAME

The GES parameter name has a general form of:

```
<identifier>(<phase>,<constituent array>;<digit>)
```

Examples of parameter names:

- `G(GAS,C1O2)`: The Gibbs energy of formation of a CO2 molecule in gas.
- `G(FCC,Fe:VA)`: The Gibbs energy of formation of fcc Fe with interstitials.
- `L(LIQ,Fe,Cr;0)`: The regular solution parameter for Fe and Cr in liquid.
- `L(LIQ,Fe,Cr;1)`: The sub-regular solution parameter.
- `TC(BCC,Fe:Va)`: The Curie temperature of bcc Fe.
- `BMAGN(BCC,Fe:Va)`: The Bohr magneton number parameter of bcc Fe.

The parameter name consists of several parts. The first is a type-identifier and these can be used:

- `G`: Standard energy parameter (Gibbs energy of formation) or for interaction parameters;

- **L**: Excess energy parameter (Gibbs energy of interaction) always used for interaction parameters;
- **TC**: Curie temperature for magnetic ordering;
- **BMAGN** or **BM**: Bohr magneton number for magnetic ordering (or Born function $\omega_{Pr,Tr}$ for aqueous solute species).
- **VO**: Molar volume at 298.15 K and 1 bar (a numeric value only);
- **VA**: Integrated thermal expansivity; $\int_{298.15}^T \alpha(T) dT$
- **VC**: High-pressure fitting parameter;
- **VK**: Isothermal compressibility.



For more information about the high pressure volume, see Lu, Selleby, and Sundman [2005]¹.



When necessary quantities as **H** (enthalpy), **S** (entropy), **V** (Volume), **F** (Helmholtz energy), etc., can be calculated from the Gibbs energy.

PHASE NAME

Specifying the **PHASE NAME** in uppercase is recommended; however, if you prefer to write it as a mixture of uppercase and lowercase, it automatically converts all lowercase to uppercase, as the GIBBS module only recognises uppercase phase names. It is important that if a phase bears a legal phase-type (among **G**, **A**, **Y**, **L**, **I**, **F** and **B**) in its phase definition (already by the **PHASE** keyword; such as **GAS:G**, **LIQUID:L**, **SLAG:L**, **IONIC-LIQ:Y**, **SPINEL:I**, **FCC_L12:F**, **HCP_D021:F**, **BCC_B2:B**, **AQUEOUS:A**), such a valid phase-type code should not be attached to the phase name when **ENTER_PARAMETER** is executed.

CONSTITUENT ARRAY

The constituent array consists of a list of constituent names. Interaction parameters have two or more constituents from the same sublattice separated by a comma. If the phase has sublattices, at least one constituent in each sublattice must be specified. The constituents in different sublattices must be given in sublattice order and are separated by a colon.

After the component array, a sub-index digit can be specified after a semicolon. This digit must be in the range 0 to 9. The interpretation of the sub-index depends on the excess energy model used for the phase. If no semicolon and digit are given, the sub-index value is assumed to be as zero.

The excess energy parameters, e.g. the regular/subregular (binary) parameter or ternary parameters, are multiplied with two or more fractions of the constituents from the same sublattice of the solution phase. These additional constituents must be given as interacting constituents (as the following prompt).



Solution phases with sublattices can have interacting constituents in each sublattice.

INTERACTION PARAMETER

An interaction parameter, which is used to describe the excess term of a quantity, must have two or more constituents that interact with each other on a specified sublattice site of the given phase. It is arbitrary which of these constituents is given as the first constituent and what is given as the interacting constituents. The software always sorts the constituents (in each sublattice) in alphabetical order when the parameter name is written as a prompt (for entering its parameter value) and when the parameter is listed (using the GIBBS commands ["LIST_PARAMETER" on page 236](#) or ["LIST_PHASE_DATA" on page 272](#)). This is important for all asymmetric interaction parameters where the sign of the interaction parameter must depend on the appearance order.

Use an asterisk* to denote that the excess interaction parameter is independent of the constituents of a specific sublattice. For example, $L(\text{FCC_L12}, \text{AL}, \text{NI} : *)$ means that the interaction parameter is for the binary interaction between constituents AL and NI on the first sublattice in the `FCC_L12` solution phase, while it is independent of all constituents on the second sublattice. An interaction parameter in the list of constituents is always added to the Gibbs energy and the asterisk * is calculated with the term of $[1 \sum y(\text{specified constituents})]$, which implies that in an A-B binary system these L parameters are identical (but in higher-order systems, these are different):

- $L(\text{phase}, A, B)$ is multiplied with $X(A) \cdot X(B)$
- $L(\text{phase}, A, *)$ is multiplied with $X(A) \cdot (1 - X(A))$
- $L(\text{phase}, B, *)$ is multiplied with $X(B) \cdot (1 - X(B))$

If you press <Enter> when you are asked for a parameter name or if you have improperly input the entire parameter name, you are asked for each of these items in the name.

1. Lu, Xiao-Gang, Malin Selleby, and Bo Sundman. 2005. "Implementation of a New Model

for Pressure Dependence of Condensed Phases in Thermo-Calc.” Calphad 29 (1): 49–55.
doi:10.1016/j.calphad.2005.04.001.

ENTER_PARAMETER



This command is for the PARROT module.




There is also a Gibbs (GES) module command with the same name.



["About the ENTER_PARAMETER Command" on page 264](#)

Use this command to enter TP-function(s) for a specific parameter for a phase interactively with this command. If there is already a parameter expression defined (for this parameter), that is deleted and replaced with newly entered one.

The entered TP-Function(s) for the parameter can be changed later with the command AMEND_PARAMETER.

| Syntax | ENTER_PARAMETER |
|-------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Parameter: <Parameter name></p> <p>As explained in "About the ENTER_PARAMETER Command" on page 264, specify a correct and complete Parameter Name, which should contain all the necessary parts of the general form:</p> <p><Identifier>(<Phase>,<Constituent array>;<Digit>)</p> <p>If a parameter name is not acceptable or <Enter>, is pressed, a message displays:</p> <p>*** Error, please re-enter each part separately</p> <p>and you are prompted for input for each required part for a parameter name.</p> |
| Options | Description or Information |
| Identifier | <p>Identifier (/X/): <G or L, or TC, or BM, or V0 or VA or VC or VK></p> <p>If this command is used one or more times, the previous value on this prompt is set as default. Press <Enter> for the same type identifier or specify a new type.</p> |
| Phase name | <p>Phase name (/ABCD/): <Phase name></p> <p>Each parameter is valid for a specific phase only. The name of that phase must be supplied (maximum 24 characters). The name can be abbreviated.</p> |
| Constituent | <p>Constituent (in sublattice # /ABC/): <Species name></p> <p>A parameter is identified by the constituents on a specified sublattice site of the given phase, the stoichiometric coefficients of which are multiplied with the parameter. The name of the constituent can be abbreviated.</p> <div>  <p>It is the species name, not the stoichiometric formula required here.</p> </div> |

| Syntax | ENTER_PARAMETER |
|-------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>If this command is used one or more times, the previous value on this prompt is set as default. Accept it by pressing <Enter> if the constituent is the same, or specify a new species name.</p> |
| Interacting constituent | <p>For phases with several sublattices, the program asks for one constituent in each sublattice.</p> <p>Interacting constituent (in sublattice # /XYZ/): <Species name></p> <p>If this command is used one or more times, the previous value on this prompt is set as default. Press <Enter> to accept it if the constituent is the same, or specify a new species name.</p> <div>  <p>To cancel the default value of the interacting constituent type <code>NONE</code> or the name of another constituent.</p> </div> <p>This question is repeated until all the interested interacting constituent(s) on a specific sublattice in the phase are specified, and finally an <Enter> is enforced.</p> |
| Degree | <p>Degree /#/ : <Degree></p> <p>Degree is model-dependent. Specify an integer number (a value from 0 through 9) as the degree of composition-dependent interaction contribution for the phase parameter. This is valid for excess energy (<code>L</code>), Curie temperature (<code>TC</code>) and Bohr magneton number (<code>BMAGN</code>), as well as for volume-related parameters (<code>VO</code>, <code>VA</code>, <code>VC</code> or <code>VK</code>).</p> <p>For binary interaction parameters, the degree is usually the power in the Redlich-Kister expression. For ternary interaction parameters, it is usually the Hillert ternary index.</p> <p>For a standard <code>G</code> parameter for a pure component (end-member) its degree should be always 0 and this prompt should not display.</p> |
| Phase parameter | <p>After this prompt, the program echoes on the screen the full TP-Function of the phase parameter.</p> <p>Low temperature limit /298.15/: <Lowest temperature limit in K></p> <p>Specify the lowest temperature limit (in Kelvin), or the lowest-pressure limit (in Pascal but entered as a negative number), for the current TP-Function.</p> <p>Function: <Definition for a function></p> <p>A TP-Function consists of terms in T and P.</p> <p>& <Continuation of the definition for the current function></p> <p>Continuation of a TP-Function definition.</p> <p>High temperature limit /6000/: <High temperature limit in K></p> <p>Specify the high temperature limit (in Kelvin), or the high-pressure limit (in Pascal; only if the <i>lowest limit</i> is entered as a negative number) for the current TP-Function.</p> <p>Any more ranges? /N/:</p> <p>Enter Y for more function(s) or N to end this command.</p> |

LIST_ALL_VARIABLES



This command is for the PARROT module.

Create a list of the values and status of all variables in the PARROT workspace on screen or in a text file. After an optimization some statistical information is also written. The correlation matrix is written if that option is chosen.

► ["SET_OUTPUT_LEVELS" on page 283.](#)

| Syntax | LIST_ALL_VARIABLES |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Output to screen or file /Screen/: <File name></p> <p>A list of the current values and status, as well statistical information (if after optimization) and the correlation matrix (optionally), for all variables is written on screen (by pressing <Enter>) or on the list file under a specific file name which can later on be opened and edited by basic text editor.</p> |
| | <p>EXAMPLE OUTPUT</p> <p>The following is the listed variables for the example TCEX36, after the first optimization when having set all variables available for optimization.</p> <pre>== OPTIMIZING VARIABLES == AVAILABLE VARIABLES ARE V1 TO V00 VAR. VALUE START VALUE SCALING FACTOR REL.STAND.DEV V1 2.03729090E+04 2.03688352E+04 2.03688352E+04 3.41524152E+00 V2 -2.94286372E+01 -2.94286372E+01 -2.94286372E+01 2.37944771E+00 V11 -2.17373936E+04 -2.18095983E+04 -2.18095983E+04 3.97086303E-02 V12 1.52107184E+01 1.51660547E+01 1.51660547E+01 5.84552327E-02 V15 2.42082351E+04 2.45139169E+04 2.45139169E+04 5.00914471E+00 V16 -8.38723972E+00 -8.83460472E+00 -8.83460472E+00 1.60961318E+01 V17 3.08916533E+03 3.15802558E+03 3.15802558E+03 9.63738108E+00 V19 2.20292586E+04 2.21385673E+04 2.21385673E+04 4.14274011E+01 V20 - 7.04217974E+00 -7.22424882E+00 -7.22424882E+00 1.00561540E+02 NUMBER OF OPTIMIZING VARIABLES : 9 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO THE SUM OF SQUARES HAS CHANGED FROM 8.00002729E+04 TO 8.00002719E+04 DEGREES OF FREEDOM 45. REDUCED SUM OF SQUARES 1.77778382E+03</pre> |

LIST_CONDITIONS



This command is for the PARROT module.

Use this command to generate a list of the current values of optimization conditions, as well the current status of listing, either on screen or in a basic text file which can be opened and edited by a text editor.

| | |
|--------|-------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | LIST_CONDITIONS |
| Prompt | Output to screen or file /Screen/: <File name> Press <Enter> to output to screen or on the list file under a specific file name. |

LIST_PARAMETER



This command is for the PARROT module.



There is also a Gibbs (GES) module command with the same name.

List the TP-function(s) of a specific parameter for a phase. You must supply the name of the phase parameter:

The parameter name: <Identifier>(<Phase>,<Constituent array>;<Digit>)



For encrypted commercial databases, you may not be able to use this command to list any retrieved parameter.

| | |
|---------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | LIST_PARAMETER |
| Prompts | <p>Parameter: <Parameter name></p> <p>Specify a correct and complete parameter name, which should contain all the necessary parts of the general form: <identifier>(<phase>,<constituent array>;<digit>)</p> <p> See "About the ENTER_PARAMETER Command" on page 264 to learn how to define the parameter name.</p> <p>If a parameter name is not acceptable or <Enter> is pressed, an error message displays:</p> <pre>*** Error, please re-enter each part separately</pre> <p>The program prompts for separate input for each required part for a parameter name.</p> |
| | <p>Identifier (/X/): <G or L, or TC, or BM, or V0 or VA or VC or VK></p> <p>Specify one of these types of legal identifiers.</p> |
| | <p>Phase name (/ABCD/): <Phase name></p> <p>Specify the phase name.</p> |
| | <p>Constituent (in sublattice # /ABC/): <Species name></p> <p>Specify the constituent name on the specified sublattice site of the given phase.</p> |

| Syntax | LIST_PARAMETER |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | Interacting constituent (in sublattice # /XYZ/): <Species name> Specify the interacting constituent name on the specified sublattice site of the given phase; if there is no interacting constituent, press <Enter>. |
| | Interacting constituent (in sublattice # /XYZ/): <Species name> If there is more than one interacting constituent on the specified sublattice site of the given phase, specify them; otherwise press <Enter>. |
| | Degree /#/ : <Degree> Specify a numerical number as the degree for the phase parameter. |

LIST_PHASE_DATA



This command is for the PARROT module.

List all the phase from the Gibbs (GES) module for a specific phase. These are displayed on screen. The thermochemical parameters listed for each phase are always in SI units.

| Syntax | LIST_PHASE_DATA |
|--------|-------------------------------------------------------|
| Prompt | Phase name: <Phase name> Specify a phase name. |

LIST_RESULT



This command is for the PARROT module.

List the result of the current optimization run on screen or in a specified file. The level of detail listed can be prescribed by the command SET_OUTPUT_LEVELS.

The LIST_RESULT command has an option **G** for creation of an experimental data file with two columns, one for the experimental value and the other for the calculated value. It allows plotting a diagram and visualizing the fitting results. The plot is automatically plotted and you can scale it giving commands in the POST module. The option **D** lists all experiments, including those with fulfilled inequalities which are suppressed with the default option **C**.

| Syntax | LIST_RESULT |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | Full, Condensed, Detailed or Graphic format: /C/: <C or D or F or G> Choose a format. <ul style="list-style-type: none"> The F (full) format is obsolete but retained for backward compatibility. C (condensed) is the default. |

| Syntax | LIST_RESULT |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <ul style="list-style-type: none"> • D (detailed) lists all experiments, including those with fulfilled inequalities (not included with the default condensed file). • The G (graphical) format creates an experimental data file containing two columns, one with the experimental value and the other with the calculated value. This allows plotting of a diagram where all symbols should be on the diagonal if the fit is perfect. The plot is automatically plotted and you can scale it giving commands in the POST module. <p>Output to screen or file /Screen/: <File name></p> <p>A list of the current optimization results are written on screen (by pressing <Enter>) or on the list file under a specific file name which can later on be opened and edited by basic text editor.</p> |
| | <p>The output normally consists of these parts:</p> <ul style="list-style-type: none"> • A title showing the data of the action; • A message on successful optimization with the iteration number in the last optimization; • A paragraph describing the optimization condition; • A list of the latest set of optimized and fixed variables; • A paragraph describing the optimization quality (some statistical information); • A correlation matrix for all optimizing variables (optionally shown, pre-set by the SET_OUTPUT_LEVELS command); • A list of all parameters (including their symbol names, status and current values or function expressions), and all phase descriptions (including phase name, model names, constituents, and phase's G/L/TC/BM expressions) predefined for each phase in the system (optionally shown, pre-set by the SET_OUTPUT_LEVELS command); • A paragraph describing the alternate equilibria (and possible error during optimization); • A detailed list on all the equilibrium points used in the current optimization. If the alternate-mode is used in the optimization, only an error value is shown. For normal-mode calculations, a list is shown for the experimental equilibrium numbers (first column) and corresponding original experimental data (second column, in the form quantity = value) which are used in optimization (i.e. non-zero weighted points). Such experimental data are by each point compared by the calculated value (third column) after the last optimization. Also listed are the experimental error (column 4), the difference between the calculated value and original experimental data (column 5), and the contribution to the sum of least square (column 6). |

EXAMPLE OUTPUT

The following is the listed result after the first optimization based on the prescribed definitions in the TCEX36a.TCM and TCEX36b.TCM, but having set all variables available for optimization.

```
=====
                OUTPUT FROM P A R R O T.

*** SUCCESSFUL OPTIMIZATION. ***          NUMBER OF ITERATIONS:  10
```

```

== OPTIMIZING CONDITIONS ==
RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 1 DMAX = 1.00000000E+02 H = 1.00000000E-04 ACC = (INITIAL
SUM OF SQUARES) * 1.00000000E-03
== OPTIMIZING VARIABLES ==
AVAILABLE VARIABLES ARE V1 TO V00

```

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|-----------------|-----------------|-----------------|----------------|
| V1 | 2.03749463E+04 | 2.03729090E+04 | 2.03729090E+04 | 3.41455863E+00 |
| V2 | -2.94286372E+01 | -2.94286372E+01 | -2.94286372E+01 | 2.37944774E+00 |
| V11 | -2.17395673E+04 | -2.17373936E+04 | -2.17373936E+04 | 3.98405298E-02 |
| V12 | 1.52107184E+01 | 1.52107184E+01 | 1.52107184E+01 | 5.82861832E-02 |
| V15 | 2.42106560E+04 | 2.42082351E+04 | 2.42082351E+04 | 5.07239609E+00 |
| V16 | -8.38723972E+00 | -8.38723972E+00 | -8.38723972E+00 | 1.69546796E+01 |
| V17 | 3.08947424E+03 | 3.08916533E+03 | 3.08916533E+03 | 9.85220694E+00 |
| V19 | 2.20314615E+04 | 2.20292586E+04 | 2.20292586E+04 | 4.16329629E+01 |
| V20 | -7.04217974E+00 | -7.04217974E+00 | -7.04217974E+00 | 1.03161466E+02 |

```

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 8.00002719E+04 TO 8.00002709E+04
DEGREES OF FREEDOM 45. REDUCED SUM OF SQUARES 1.77778380E+03
Number of alternate equilibria 14

```

| SYMBOL | STATUS | VALUE/FUNCTION |
|--------|----------|------------------|
| R | 80000000 | 8.3145100E+00 |
| RTLNP | 20000000 | +R*T*LN(1E-05*P) |
| V1 | 48000000 | 2.0374946E+04 |
| V2 | 48000000 | -2.9428637E+01 |
| V11 | 48000000 | -2.1739567E+04 |
| V12 | 48000000 | 1.5210718E+01 |
| V15 | 48000000 | 2.4210656E+04 |
| V16 | 48000000 | -8.3872397E+00 |
| V17 | 48000000 | 3.0894742E+03 |
| 21 V19 | 48000000 | 2.2031462E+04 |
| 22 V20 | 48000000 | -7.0421797E+00 |

```

LIQUID

```

EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
A,B

CONSTITUENTS:

$G(\text{LIQUID}, A; 0) - G(\text{BCC}, A; 0) = 500.00 < T < 2000.00: +14000 - 10 * T$
 $G(\text{LIQUID}, B; 0) - G(\text{BCC}, B; 0) = 500.00 < T < 2000.00: +18000 - 12 * T$
 $L(\text{LIQUID}, A, B; 0) = 500.00 < T < 2000.00: +V11 + V12 * T$
 $L(\text{LIQUID}, A, B; 1) = 500.00 < T < 2000.00: +V13 + V14 * T$

A2B

2 SUBLATTICES, SITES 2: 1 CONSTITUENTS: A : B

$G(\text{A2B}, A; B; 0) - 2 G(\text{BCC}, A; 0) - G(\text{BCC}, B; 0) =$
 $500.00 < T < 2000.00: +V1 + V2 * T + V3 * T * \text{LN}(T)$

BCC

EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
A,B

CONSTITUENTS:

$G(\text{BCC}, A; 0) - G(\text{BCC}, A; 0) = 500.00 < T < 2000.00: 0.0$
 $G(\text{BCC}, B; 0) - G(\text{BCC}, B; 0) = 500.00 < T < 2000.00: 0.0$
 $L(\text{BCC}, A, B; 0) = 500.00 < T < 2000.00: +V15 + V16 * T$
 $L(\text{BCC}, A, B; 1) = 500.00 < T < 2000.00: +V17 + V18 * T$

FCC

EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
A,B

CONSTITUENTS:

$G(\text{FCC}, A; 0) - G(\text{BCC}, A; 0) = 500.00 < T < 2000.00: 408$
 $G(\text{FCC}, B; 0) - G(\text{BCC}, B; 0) = 500.00 < T < 2000.00: +3300 - 3 * T$
 $L(\text{FCC}, A, B; 0) = 500.00 < T < 2000.00: +V19 + V20 * T$
 $L(\text{FCC}, A, B; 1) = 500.00 < T < 2000.00: +V21 + V22 * T$

===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, PO=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

| | |
|-----------------------------------|------------|
| Alternate equilibrium calculation | 0.4183 |
| Alternate equilibrium calculation | 0.1932 |
| Alternate equilibrium calculation | 0.1016 |
| Alternate equilibrium calculation | 1.4354E-03 |
| Alternate equilibrium calculation | 2.5063E-02 |
| Alternate equilibrium calculation | 8.3929E-03 |
| Alternate equilibrium calculation | 141.4 |
| Alternate equilibrium calculation | 141.4 |

| | | | | | |
|-----------------------------------|--------|------------|-------------|-------------|---------|
| Alternate equilibrium calculation | | 141.4 | | | |
| Alternate equilibrium calculation | | 141.4 | | | |
| Alternate equilibrium calculation | | 1.2532E-03 | | | |
| Alternate equilibrium calculation | | 5.4781E-04 | | | |
| Alternate equilibrium calculation | | 1.5404E-03 | | | |
| Alternate equilibrium calculation | | 1.2702E-03 | | | |
| ACR(B)=9.4E-1 | 0.9397 | 2.85E-02 | -2.7745E-04 | -9.7472E-03 | |
| ACR(B)=8.4E-1 | 0.8395 | 2.82E-02 | -4.9038E-04 | -1.7396E-02 | |
| ACR(B)=7.4E-1 | 0.7407 | 2.81E-02 | 7.3804E-04 | 2.6305E-02 | |
| ACR(B)=6.4E-1 | 0.6424 | 2.81E-02 | 2.3935E-03 | 8.5272E-02 | |
| ACR(B)=5.4E-1 | 0.5434 | 2.82E-02 | 3.4449E-03 | 0.1220 | |
| ACR(B)=4.4E-1 | 0.4428 | 2.85E-02 | 2.8265E-03 | 9.9024E-02 | |
| ACR(B)=3.4E-1 | 0.3394 | 2.90E-02 | -5.8174E-04 | -2.0040E-02 | |
| ACR(B)=2.3E-1 | 0.2320 | 2.97E-02 | 2.0260E-03 | 6.8208E-02 | |
| ACR(B)=1.2E-1 | 0.1194 | 3.06E-02 | -6.4192E-04 | -2.0981E-02 | |
| HMR(LIQUID)=-1964 | -1957. | 5.00E+02 | 7.439 | 1.4878E-02 | |
| HMR(LIQUID)=-3500 | -3478. | 5.00E+02 | 21.67 | 4.3338E-02 | |
| HMR(LIQUID)=-4588 | -4565. | 5.00E+02 | 22.69 | 4.5382E-02 | |
| HMR(LIQUID)=-5239 | -5217. | 5.00E+02 | 21.50 | 4.3008E-02 | |
| HMR(LIQUID)=-5454 | -5435. | 5.00E+02 | 19.11 | 3.8216E-02 | |
| HMR(LIQUID)=-5233 | -5217. | 5.00E+02 | 15.50 | 3.1008E-02 | |
| HMR(LIQUID)=-4575 | -4565. | 5.00E+02 | 9.691 | 1.9382E-02 | |
| HMR(LIQUID)=-3481 | -3478. | 5.00E+02 | 2.669 | 5.3385E-03 | 118 HMR |
| (LIQUID)=-1950 | -1957. | 5.00E+02 | -6.561 | -1.3122E-02 | |

LIST_STORE_FILE



This command is for the PARROT module.

Use the LIST_STORE_FILE command to display the name of the store file and its full path.


LIST_SYMBOL_IN_GES



This command is for the PARROT module.

Lists TP-function(s) for the entered model parameters for phases in the system on screen. In many cases, the optimizing variables are parts of the TP-functions which in turn are entered in model parameters for various phases in the GIBBS workspace.

This command is a way to find out how the functions depend on the optimizing variables. In the PARROT module the list is only shown on screen, not written to any file (which the LIST_SYMBOL command in the GIBBS module does).


| Syntax | LIST_SYMBOL_IN_GES |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Name: <Symbol name></p> <p>Specify a symbol name.</p> <div>  <p>Only those symbols that match this name are listed. Or press <Enter> for a list of all available symbols entered in the system.</p> </div> |

OPTIMIZE_VARIABLES



This command is for the PARROT module.

Perform variable optimization. All system-definition data needed for the optimization is read from the current work file (*.PAR). The result of the optimization is automatically stored in the current work file.

| Syntax | OPTIMIZE_VARIABLES |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Number of iteration /N/: <Integral number of iteration></p> <p>Specify an integral number for the optimization iteration. The specified iteration number is shown as the default number. The PARROT module tries this number of different sets of values of the optimizing variables unless it has converged earlier, or has given up earlier.</p> <div>  <p>It initially takes a small step in each variable to find the steepest slope. You can give zero iteration to calculate the error in all selected experiments, and then use LIST_RESULT to check how good (bad) the current fit is.</p> </div> |

READ_PARROT_WORKSPACES




This command is for the PARROT module.

► ["Workspace Files" on page 26](#)

Read the previous PARROT/GIBBS/POLY workspaces back to replace the current PARROT/GIBBS/POLY workspaces. It is useful if late changes made through various PARROT/GIBBS/POLY commands are not satisfactory.

| Syntax | READ_PARROT_WORKSPACES |
|--------|--------------------------------------------------------------------------------------------------|
| | The previous PARROT/GIBBS/POLY workspaces are always associated with the latest action to either |

| Syntax | READ_PARROT_WORKSPACES |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | open a work file by SET_STORE_FILE, or to create a work file by CREATE_NEW_STORE_FILE (either interactively in the PARROT module or through a MACRO_FILE_OPEN of an *SETUP.TCM file), or to update the work file by SAVE_PARROT_WORKSPACES. |
| | Unlike the READ commands in other modules (e.g. GIBBS or PLOY), this command in the PARROT module does not ask for the file name where to read a previously opened/created/updated PARROT/GIBBS/POLY workspaces, for the reason described above. |
| |  You cannot use this command if there is no work file opened or created already. |

RECOVER_VARIABLES

The RECOVER_VARIABLES command is used to set back the values of all variable to the start values.

REINITIATE



This command should not be used unless you want to destroy the current PARROT workspace. However, this PARROT command does not reinitiate the GIBBS/POLY3 workspaces.



This command is for the PARROT module.

The REINITIATE command is used to reinitiate the workspace used by PARROT. All output and optimizing conditions are given their default values. All variables are set fixed with their value equal to zero.

RESCALE_VARIABLES

When using the RESCALE_VARIABLES command, the current values of all the parameters are copied to their start values and the scaling factors for further optimization. Thus it should be done now and again, in particular if you think the optimization results are improved after the previous run(s), or if any variable changes more than a factor of 10.

SAVE_PARROT_WORKSPACES




This command is for the PARROT module.

If the latest changes made through various PARROT/GIBBS/POLY commands are as required, use this command to save the current workspace (i.e. data area) used by the PARROT program (also including the current GIBBS and POLY workspaces), onto the present work *.PAR file which has already been opened by SET_STORE_FILE or been created by CREATE_NEW_STORE_FILE (either interactively in the PARROT module or through a MACRO_FILE_OPEN of an *SETUP.TCM file).



The PARROT/GIBBS/POLY workspaces are updated after each PARROT/GIBBS/POLY command. This means the current PARROT/GIBBS/POLY workspaces are always updated onto the latest work *.PAR file that is associated with the latest SET_STORE_FILE or CREATE_NEW_STORE_FILE command.

▶ ["Workspace Files" on page 26](#)

| Syntax | SAVE_PARROT_WORKSPACE |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| |  <p>Unlike the SAVE commands in other modules (e.g. GIBBS or PLOY), this command in the PARROT module does not ask for the file name where to save the current PARROT/GIBBS/POLY workspaces, for the reason described above. You cannot use this command if there is no work *.PAR file opened or created already.</p> |

SET_ALTERNATE_MODE

Turn the alternate mode on or off.

With the ALTERNATE mode is possible to include functions to be evaluated together with an alternate calculation and to select ALTERNATE mode for each experimental equilibrium.



The alternate mode is described in ["About Alternate Mode" on page 49](#). It should be used only to optimize start values of the model parameters in the beginning of the assessment.

| Syntax | SET_ALTERNATE_MODE |
|--------|--------------------------------------------------------|
| Prompt | <p>On /Y/:</p> <p>By default alternate mode is ON.</p> |

SET_EXTERNAL_PARAMETER



This command is for the PARROT module.

Optimize model parameters of the so-called external models, which may not be as fully-implemented/integrated parts inside the GIBBS system and thus are independently defined within user-specified/written source codes. This command makes links between the PARROT optimizing variables and external model parameters.



In order to be able to build the specified external model and to use this SET_EXTERNAL_PARAMETER command, it requires you to first write codes for a preferred external model (as it is not within the standard GIBBS system of the Thermo-Calc software) and then provide it to a consultant at Thermo-Calc Software AB for the purpose of including the external model in a separate DLL that is interactively connected to the software. For more information about our consultancy services, see our [Consultancy](#) page on our website.

| Syntax | SET_EXTERNAL_PARAMETER |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>External name: <Parameter name in the external model></p> <p>Correctly specify the parameter name defined within a specified/written external model.</p> |
| | <p>As optimizing variable number: <n></p> <p>Give the number of the PARROT optimizing variable, which should have a unique link to the specified parameter name of the external model.</p> <p>For example, @@ Link PARROT variables to CAM parameters:</p> <pre>SET-EXTER-PAR GT (SLAG_A,O-2,SI+4,CA+2) 1 SET-EXTER-PAR ET (SLAG_A,O-2,SI+4,CA+2) 2 SET-EXTER-PAR EXT (SLAG_A,O-2,SI+4,CA+2) 3</pre> |

SET_FIX_VARIABLE

Prescribe a fixed value to a variable. The variable is considered as a constant at the optimization, usually after successful optimization runs for some specific variables (for some of the phases in the system). Such fixed variables can also be set back for further optimization run by using SET_OPTIMIZING_VARIABLE.

| Syntax | SET_FIX_VARIABLE |
|---------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Variable number: <Variable number(s)></p> <p>Specify the number of the variable. It is possible to give a range by giving two numbers with a hyphen in between (no spaces allowed), e.g. 1. The parameters within the limits are set fixed to their current values (no question of values).</p> |
| | <p>Start value /xxxx.xxxxx/: <A value to be fixed></p> <p>Specify a numerical value to be fixed for the selected variable (only when one variable number is</p> |

| | |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | SET_FIX_VARIABLE |
| | <p>specified at the previous prompt). The current value for the selected variable is shown as default.</p> <p>If a range of variable numbers is specified at the previous prompt, this question is not prompted, and the current values are used as fixed values.</p> |

SET_OPTIMIZING_CONDITION




This command is for the PARROT module.

Specify the conditions for the optimization. The default values are chosen automatically by the PARROT program, and in most cases these should not be changed.



The optimization stops when the sum of errors decreases by this value, even though it might be possible to increase it further with a new OPTIMIZE command.

| | |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | SET_OPTIMIZING_CONDITION |
| | <p>Relative standard deviation for experiments? /N/:</p> <p>By default the standard deviation of the experimental determinations are absolute values. Enter Y if these are used as relative weighting factors.</p> <div>  <p>The estimated standard deviations of the optimized variables might be different for the two cases.</p> </div> |
| Prompt | <p>Min save on file? /Y/:</p> <p>Specify whether the program should minimize the transfer of data to and from the current work file during the optimization:</p> <ul style="list-style-type: none"> • If the default (N) is kept, the workspaces are stored on the current work file after every iteration in the optimization procedure. • Enter Y to speed up the optimization. After optimization use the SAVE_PARROT_WORKSPACES command to update the progress onto the current work file. |
| | <p>Relative step for calculation of derivatives: /1e-04/: <xxx></p> <p>In the calculation of the correlation matrix for equilibria with inaccuracy in the independent state variables, some numerical derivatives might have to be calculated.</p> <p>Specify the relative step (xxx) for the calculation of these derivatives.</p> |
| | <p>Maxfun (va05ad): /100/: <n></p> <p>The maximum number of iterations in the optimization. The same value set by the OPTIMIZE command.</p> |
| | <p>Dmax (va05ad): /100/: <n></p> |

| Syntax | SET_OPTIMIZING_CONDITION |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | An estimate of the maximum distance between the start and the final values of the variables. A smaller value makes the program vary the parameters with smaller factors. |
| | H (va05ad): /1e-04/: <xxx> The step used in the scaled variables for calculating numerical derivatives during the optimization. |
| | Acc/(initial sum of squares) (va05ad): /.001/: <xxx> The break condition for the optimization. The accepted value is the difference between the true minimum and the calculated one. |

SET_OPTIMIZING_VARIABLE



This command is for the PARROT module.

Specify which variable value should be estimated at the optimization. Such a variable can have a value of zero or another start value, or is fixed by SET_FIX_VARIABLE prior to the previous optimization run.

For a good reference prior to this command, a list of all variables (which are used to define various parameters for phases in the optimizing system, as pre-entered in the *SETUP.TCM file or interactively entered in the GIBBS module) are obtained by using LIST_ALL_VARIABLES.

| Syntax | SET_OPTIMIZING_VARIABLE |
|---------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Variable number: <Variable number(s)></p> <p>Specify the number(s) for the variable(s) to be set. Any non-zero parameter within the range is allowed to be optimized. A parameter with a current value equal to zero must be specified explicitly here in order to be optimized.</p> <p>Specify a range by giving two numbers connected by a hyphen (no space allowed!), e.g. 2-8. Under this circumstance, no question of start values are asked.</p> |
| | <p>Start value /xxxx.xxxxx/: <A guess value></p> <p>Specify a start guess of the optimum value (only when one variable number is specified at the previous prompt). The current numerical value for the selected variable is shown as default.</p> <div> <p>This guess is critical as the initial guess of all parameters must make it possible to calculate the selected equilibria. If a range of variable numbers is specified at the previous prompt, this question is not prompted, and the current values (as start values) are not changed.</p> </div> |

SET_OUTPUT_LEVELS



This command is for the PARROT module.

Choose the type of information the PARROT module gives during the optimization procedure and when listing results.


| Syntax | SET_OUTPUT_LEVELS |
|---------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | List increment /1/: <Increment in iteration number> Specify the increment in iteration number for which information is listed on screen during the optimization. By giving a larger number it shortens the list. |
| | List sum of squares: /Y/: Choose whether the sum of squares is listed on screen during the optimization procedure. |
| | List scaled variables: /Y/: Choose whether the scaled variable values are listed on the terminal during the optimization procedure. |
| | List weighted residuals: /N/: Choose whether the weighted residuals are listed on the terminal during the optimization procedure. |
| | List all parameters: /N/: Choose whether all parameters in the models are listed in LIST_RESULT. |
| | List correlation matrix: /N/: Choose whether the correlation matrix of the variables are listed with the commands LIST_RESULT and LIST_ALL_VARIABLES. |

SET_SCALED_VARIABLE

This command is similar to SET_OPTIMIZING_VARIABLE in that it specifies start values for optimizing variables. The difference being it is functional for only one optimizing variable at one time. It also prescribes a minimum and maximum value for the variable. During the optimization runs, the variable value is limited within this min-max range.

Such a variable may have a value of zero or another start value, or may be fixed by SET_FIX_VARIABLE prior to the previous optimization run. For a good reference prior to using this command, a list of all variables (which are used to define various parameters for phases in the optimizing system, as entered in the *SETUP.TCM file or interactively entered in the GIBBS module) is obtained by using LIST_ALL_VARIABLES.

| Syntax | SET_SCALED_VARIABLE |
|---------|---------------------------------------|
| Prompts | Variable number: <Variable number(s)> |

| Syntax | SET_SCALED_VARIABLE |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | Specify the number for an optimizing variable to be set. Any non-zero parameter is allowed to be optimized, and a parameter with a current value equal to zero must be specified explicitly here in order to be optimized. |
| | <p>Start value /xxxx.xxxxx/: <A guess value></p> <p>Specify a start guess of the optimum value. The current numerical value for the selected variable is shown as default.</p> <div>  <p>This guess is critical as the initial guess of all parameters must make it possible to calculate the selected equilibria.</p> </div> |
| | <p>Min value /xxxx.xxxxx/: <A guess value></p> <p>Specify a minimum guess of the optimum value. It should be smaller than, at least equal to, the current start value for the selected variable.</p> |
| | <p>Max value /xxxx.xxxxx/: <A guess value></p> <p>Specify a maximum guess of the optimum value. It should be larger than, at least equal to, the current start value for the selected variable.</p> |

SET_STORE_FILE



This command is for the PARROT module.

Specify a store file (work file) to be used for compilation and optimization. The *.PAR work file must be created (CREATE_NEW_STORE_FILE) as a store file. The GIBBS, POLY and PARROT workspaces are read from the specified store file (with a default extension of PAR).

| Syntax | SET_STORE_FILE |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | Enter a *.PAR file name in the File name field and specify the working directory in the Look in field. Normally the default file-type in the Files of type field is the correct one for the PARROT workspace format (i.e. *.PAR file). Click Open or Cancel as applicable. |

EDIT_EXPERIMENTS (ED_EXP) Submodule Commands



["EDIT_EXPERIMENTS" on page 263](#) (ED-EXP) is a submodule of PARROT.

In this section:

| | |
|------------------------------|-----|
| ADVANCED_OPTIONS | 287 |
| CHANGE_STATUS | 287 |
| COMMENT | 291 |
| COMPUTE_ALL_EQUILIBRIA | 291 |
| CREATE_NEW_EQUILIBRIUM | 292 |
| DEFINE_COMPONENTS | 293 |
| DELETE_SYMBOL | 293 |
| ENTER_SYMBOL | 294 |
| EVALUATE_FUNCTIONS | 296 |
| EXPERIMENT | 296 |
| EXPORT | 298 |
| FLUSH_BUFFER | 298 |
| GRAPHICS_PLOT | 299 |
| IMPORT | 299 |
| LABEL_DATA | 300 |
| LIST_ALL_EQUILIBRIA | 300 |
| LIST_CONDITIONS | 301 |
| LIST_EQUILIBRIUM | 301 |
| LIST_STATUS | 302 |
| LIST_SYMBOLS | 303 |
| MAKE_POP_FILE | 303 |
| READ_WORKSPACES | 304 |

| | |
|----------------------------------------------|-----|
| REINITIATE_MODULE | 304 |
| RESTORE_ALL_WEIGHTS | 305 |
| SAVE_WORKSPACES | 305 |
| SELECT_EQUILIBRIUM | 306 |
| SET_ALL_START_VALUES | 306 |
| SET_ALTERNATE_CONDITION | 307 |
| SET_CONDITION | 310 |
| SET_NUMERICAL_LIMITS | 312 |
| SET_REFERENCE_STATE | 313 |
| SET_START_CONSTITUTION | 315 |
| SET_START_VALUE | 315 |
| SET_WEIGHT | 316 |
| SHOW_VALUE | 317 |
| STORE_ALL_WEIGHTS | 318 |
| TABLE_HEAD, TABLE_VALUES and TABLE_END | 318 |
| TRANSFER_START_VALUES | 320 |

ADVANCED_OPTIONS



This command is available with the POLY and ED-EXP modules.



["ADVANCED_OPTIONS" on page 135](#) described for the POLY module.

| | |
|--------|----------------------------------------|
| Syntax | ADVANCED_OPTIONS |
| Prompt | Which option? /Step_and_Map/: <Option> |

CHANGE_STATUS



This command is available with the POLY and ED-EXP modules.

In the POLY module, set the status for components, species and phases in the defined system for all the sequential calculations (single-point, stepping and mapping) in equilibrium or local/partial equilibrium state. Each component, species and phase has a status. The default status is `ENTERED`.

The most important use is to calculate metastable equilibria and metastable phase diagrams by setting some phases (that would otherwise be stable) to the `SUSPENDED` or `DORMANT` phase-status. Another important applications is to calculate paraequilibria by setting some components to the `SPECIAL` component-status.

For a component and for a species, the status can be one of the following:

- `ENTERED`: the component(s) or species are included in the calculation. This is the default status.
- `SUSPENDED`: the component(s) or species are not considered in the calculation.
- `SPECIAL`: the specified component(s) are not included in summations for mole or mass fractions. It only works for component(s).



Only component(s) can have the status `SPECIAL`, which implies that these are not included in summations for mole or mass fractions.

For example, for the *u-fractions* or other normalized fractions, when one or more of the components are excluded from the summation, you must specify which component(s) should be excluded from the calculation of mole or mass fraction. This component status is particularly useful when calculating paraequilibrium states. Such component(s) are normally interstitial component, and must have the status `SPECIAL`. This is assigned by the `CHANGE_STATUS` command.

| Syntax | CHANGE_STATUS |
|---------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>For phases, species or components? /Phases/: <Keyword></p> <p>Keyword = phase or species or components</p> |
| | <p>Phase name(s): <Name(s) of the phase(s)></p> <p>For phase as the keyword, the names of the phases that have their status changed must be given (all on one line). A comma or space must be used as separator. The status to be assigned to the phases can also be given on the same line if preceded with an equal sign (=).</p> <p> An asterisk, *, can be used to denote all phases. The special notations *S, i.e. a wildcard * directly followed by an S, sign, means all suspended phases. In the same way, *D means all dormant phases, and *E means all entered phases.</p> |
| | <p>Name(s): <Name(s) of the Species or Component(s)></p> <p>For species or components as the keyword, the names of the species or components that have their status changed must be given (all on one line). A comma or space must be used as separator. Similarly to the case of phase as the keyword, the status to be assigned to the species or components can also be given on the same line if preceded with an equal sign =.</p> <p> An asterisk, *, can be used to denote all species or components. The special notations *S, i.e. a wildcard * directly followed by an S, sign, means all suspended species or components. In the same way, *E means all entered species or components.</p> |
| | <p>Status /Entered/: <New status></p> <p>The new status to be assigned must be given.</p> <p>For species, the values ENTERED or SUSPENDED can be used.</p> <p>For components, the status ENTERED, SUSPENDED or SPECIAL can be given. SPECIAL means that this component is excluded from sums for mole fractions and mass fractions, which is useful when calculating the <i>ufractions</i> or other normalized fractions of system components.</p> <p>For phases, the status ENTERED, SUSPENDED, DORMANT or FIXED can be given. DORMANT means the same as suspended but the driving force is calculated. FIXED means that it is a condition that the phase is stable at a certain amount.</p> <p>For example, for the <i>ufractions</i>, when one or more of the components are excluded from the summation, you must specify which component should be excluded from the calculation of the mole fraction. This component must have the status SPECIAL. This is assigned by the CHANGE_STATUS command: Change_Status comp C=special.</p> |
| | <p>Start value, number of mole formula units /0/: <Initial amount></p> <p>For ENTERED phases, an initial amount of the phase can be given. Normally, 0 is given if the phase is not likely to be stable, and 0.5 or 1 or any positive number if the phase could be stable, but such an initial amount is only used as the rough starting estimation in the equilibrium calculations.</p> |

Syntax

CHANGE_STATUS

Number of mole formula units /0/: <Equilibrium amount>

For FIXED phases, the equilibrium amount of the phase [always using an initial estimation being the $NPF(\text{phase})$ value which it is the normalized mole number of components (per mole formula unit) of the specific status-fixed phase] must be given. If the equilibrium amount is zero, then the phase is at its stability limit.

Note when specifying a FIXED phase status

Special attention should be paid when specifying a FIXED phase status in equilibrium calculations (for single points, stepping or mapping calculations), as described below.

The phase amount variables, $NP(\text{phase})$, $BP(\text{phase})$ and $VP(\text{phase})$, as well as all their M/W/V-suffixed quantities, should not be used as conditions. Instead, use the CHANGE_STATUS command to set a relevant condition, e.g. `CHANGE_STATUS phase <phase>=fix <amount>` where the fixed <amount> is roughly the same as the F-suffixed quantity $NPF(\text{phase})$.

The $NPF(\text{phase})$ quantity is the normalized mole number of components (per mole formula unit) of the specific phase in the defined system, which unlike other F-suffixed state variables [e.g. $GF(\text{phase})$, $HF(\text{phase})$ and $DGF(\text{phase})$] cannot be directly applied in any POLY command, implying that it cannot be directly evaluated or listed/shown. If intended to shown such a normalized phase amount value in an equilibrium state, you should use a properly-entered symbol (function or variable), for example: $NPF_{abc} = NP(abc) / NA$ or $NPF_{abc} = NPM(abc) / NA * N$. N is the total system size (in mole). The NA value is a quantity that is phase-dependent (and sometimes also equilibrium-dependent for ionic solution phases), and is the total atomic number in a mole-formula-unit of the specific phase abc (excluding interstitial component and, of course, vacancy). For example, the SIGMA, FCC, BCC and LIQUID phases (among others) in a defined Fe-Cr-Ni-C-N-O system (retrieved from a specific database) may be modeled by certain models, and their NA values must be evaluated in different ways, as described below:

```
LIQUID (C,Cr,CrO3/2,Fe,FeO,FeO3/2,N,Ni,NiO)1 NA = 1
FCC_A1 (Cr,Fe,Ni)1 (Va,C,N,O)1 NA = 1
BCC_A2 (Cr,Fe,Ni)1 (Va,C,N,O)3 NA = 1
SIGMA (Fe,Ni)8 (Cr)4 (Cr,Fe,Ni)18 NA = 30
```

If in the same Fe-Cr-Ni-C-N-O system the liquid solution phase is modeled by the Two-Sublattice Ionic Liquid Model, i.e.:

```
IONIC_LIQ (Cr+3,Fe+2,Ni+2)p (VA,C,N,O-2,FeO3/2)q,7
```

then the evaluation of its NA value becomes even more complicated:

$$NA = p + q * y_{C2} + q * y_{N2} + q * y_{O2} + q * y_{FeO2} + q * y_{FeO2} / 2$$

where the stoichiometric coefficients p and q are also dependent upon the real equilibrium state (rather than having fixed values in the system). Similar situations occur for other (solid) phases which are described by a multiple sublattice model with ionic constituents, such as SPINEL and HALITE phases in some databases.

There is no strange thing when using a zero value [i.e. 0] in a FIXED phase-status, since it means the specified phase is stable in equilibrium state but has a zero-amount of mass in the equilibrium calculations; in other words, on a phase diagram, the specific phase is on a zero-fraction line (ZFL), i.e. it starts becoming stable on one side of a corresponding phase-boundary line or unstable on

| Syntax | CHANGE_STATUS |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>the other side of the same boundary. It is often and efficient to do so when calculating e.g. solidus equilibrium states.</p> <p>However, when a non-zero value [it must always be positive; e.g. 1 or 0.5 or 0.3 or 1.5] is to be specified in a FIXED phase-status, it is unnecessarily the exactly same stable amount of the specific FIXED-status phase in a calculated equilibrium state any longer; instead, the <equilibrium amount> value is the NPF(phase) value that is only roughly used as the estimated starting-value of the FIXED-status phase in the equilibrium calculations.</p> <p>Therefore, a FIXED-status for a liquid phase being unity does not necessarily imply that it is a liquidus equilibrium state (where the liquid phase is in equilibrium with some solid phases but the liquid phase takes all the mass in the defined system). A unity value for setting the liquid phase status in calculating liquidus equilibrium state can only be used when the liquid mixture phase is predefined as a single-sublattice solution phase (such as metallic liquid phase in multicomponent alloy systems) and the total system size as one mole (i.e. N=1).</p> <p>When a phase is described by a solution model in which two or more sublattices are considered and these sublattice sites may also have different stoichiometric coefficients [meaning that the mixture phase could have more than one atom in formula [NA>1; see some examples above], the unity value should not be used when setting the FIXED status for the phase; instead, you should use an appropriate value that ranges from 0 to a NPF(phase) value that equals to or is smaller than 1/NA (if the total system size N=1) or 1/NA*N (if N differs from unity). For this reason, if a multicomponent system bears an IONIC_LIQUID phase that is described by the Two-Sublattice Ionic Liquid Model (or any other multiple-sublattice ionic solution phases), it is difficult to use a proper NPF(ION_LIQ) value in setting its FIXED phase-status, because that should be less than (or equal to) the complex value of</p> $N/[p + q \cdot y_{C2} + q \cdot y_{N2} + q \cdot y_{O2} + q \cdot y_{FeO}^{2/3}].$ |

EXAMPLES

For example, to obtain the metallic fraction in a system with carbon as an interstitial component, you can set the component status for carbon as `SPECIAL`:

```
Change_Status comp C=special
```



The `SUSPENDED` status for components and species does not always work as expected.

For a phase, it may have one of these statuses:

- **ENTERED:** the phase(s) are included in the equilibrium calculations and these are stable if that minimizes the total Gibbs energy in the defined system. This is the default status for all phases already retrieved from the chosen database(s). An ENTERED phase-status is always associated with an initially-estimated amount [in

mole number; normally, as 0 if the phase is not likely to be stable, and as 0.5 or 1 or any positive number if the phase could be stable] but it is only used as the rough starting value in the equilibrium calculations.

- **SUSPENDED:** the phase(s) are not considered in the equilibrium calculations.
- **DORMANT:** the phase(s) are not considered in the equilibrium calculations but their driving forces for precipitation are calculated.
- **FIXED:** it is an equilibrium condition that the status-fixed phase must be stable, and be in equilibrium at a specified amount [always using an initial estimation being the $NPF(\text{phase})$ value which it is the normalized mole number of components (per mole formula unit) of the specific status-fixed phase]. See more descriptions at the end of this command.

COMMENT



This command is for the ED-EXP module.

The COMMENT command is only used in the *.POP/*.DOP files (so can be included with experimental data files) to write brief comments or descriptive information on a newly created equilibrium (experimental) data point or a set of points given in a table.

A comment can have a maximum of about 60 characters written on the same line.

COMPUTE_ALL_EQUILIBRIA



This command is for the ED-EXP module.

In ED_EXP and PARROT modules, each experiment is treated as an individual equilibrium with some measured values. These are created with CREATE_NEW_EQUILIBRIUM, and stored in an experimental data *.POP file and then compiled and saved in the POLY workspace of a PARROT work *.PAR file.



In the DICTRA module, you work with a .DOP file instead of a .POP file.

With COMPUTE-ALL-EQUILIBRIA, all equilibria from the current to the last experimental points are calculated. If an equilibrium calculation fails, the calculation is stopped at that equilibrium. Equilibria with weight zero is skipped.



A current or present experimental point means the latest selected or calculated one. Once used the current point turns to the last point in the data block; in such a case you first use SELECT_EQUILIBRIUM so that the current point is switched to a desired one.

For this command there is always a list output on screen, which consists of six columns for all experimental points available in the current data block:

- The first column is the *equilibrium identifier* (a number) assigned by this command,
- the second the *data label* assigned with LABEL_DATA,
- the third the *number of iterations*,
- the fourth the *current weight*, and
- the fifth the *current temperature*.
- In the sixth column the *fixed stable phases* are listed together with any *comment text* given after a COMMENT in the *.POP or *.DOP file.


If the weight is zero for an equilibrium columns 3-5 are replaced by the text *<unused>*. If the alternate mode is used for some experimental points, the listing is slightly different for such points. The 3-4 columns are displayed with *alt*, instead. If an alternate calculation is failed at one experimental point, the point is automatically assigned with a zero weight, and a warning message is shown above the data line (with all six columns).

CREATE_NEW_EQUILIBRIUM



This command is available with the POLY and ED-EXP modules.

During data-assessments using the ED_EXP module (a submodule of PARROT), you can, in the POLY module, create several equilibria with different sets of conditions and phases (but normally with the same set of components). By default, there is one equilibrium. To keep the set of conditions and phase for this equilibrium, create another one using this command, and use another set of conditions for that. Two equilibria may be useful to calculate easily the enthalpy difference between two states. In the PARROT module, the experimental information is stored as a sequence of equilibria.

| Syntax | CREATE_NEW_EQUILIBRIUM |
|---------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Equilibrium number /2/: <A new equilibrium number></p> <p>Each equilibrium in the POLY workspace is identified by a unique integer number. Such an equilibrium number can be recalled with SELECT_EQUILIBRIUM.</p> |
| | <p>Initiation code /2/:</p> <p>When an equilibrium is created, you can choose to ENTER all components and phases (initiation code 2), ENTER the components only (initiation code 1) or SUSPEND everything (initiation code 0). No other values are legal.</p> <div> The entered components and phases can later be changed with CHANGE_STATUS.</div> |

DEFINE_COMPONENTS





This command is available with the POLY and ED-EXP modules.

Change the set of components. By default, the elements are used as components. The set of components can be important because some conditions are set using components, for example, the amounts, activities or chemical potentials.

For example, in the system Fe-Si-O, you can define FEO, FE2O3 and SIO2 as components, thus replacing the default FE, SI and O.



This implies a command REINITIATE_MODULE and it should be given as the first command in the POLY module.

| Syntax | DEFINE_COMPONENTS |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Give all new components / existing components/: <New components></p> <p>The new components must be specified all on one line. These replace the existing component definitions.</p> <p> The number of components cannot be changed with this command. Use CHANGE_STATUS instead.</p> <p>To keep some existing components, it is recommended that you also enter these on the line. Otherwise, the added new components may not be defined correctly. This is especially important if some components are built out of several elements.</p> <p> The new components do not have to be present as species.</p> |

DELETE_SYMBOL



This command is available with the POLY and ED-EXP modules.

Use the DELETE_SYMBOL command to remove symbols i.e. constants, variables, functions or tables.

| Syntax | DELETE_SYMBOL |
|--------|--------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Name: <Name of a symbol></p> <p>Specify the name of the symbol to be deleted. Only one symbol can be deleted each time.</p> |

ENTER_SYMBOL





This command is for the ED-EXP module.



The GES, POLY and POST modules also have a command with the same name.

Symbols are a useful feature modules to define quantities that are convenient. Symbols can be constants, variables, functions or tables.

| Syntax | ENTER_SYMBOL |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Constant, Variable, Function or Table? /Function/: <Keyword></p> <p>The Keyword can be specified as CONSTANT, VARIABLE, FUNCTION or TABLE.</p> <ul style="list-style-type: none">• CONSTANTS can only be entered once and is a means of using a name for a numeric value. For example, the value of 1 atmosphere in Pascal can be denoted by <code>P0</code> after the command <code>ENTER_CONSTANT P0=101325</code>. Defined constants can be used as values in condition assignments, for example, <code>SET-COND P=P0</code>.• FUNCTIONS are expressions of state variables or other functions. These expressions are saved, and whenever a function value is requested all functions are evaluated. The reason for this is that they may depend on each other.• VARIABLES are similar to functions because they can also be expressions of state variables. However, contrary to functions, they are only evaluated when they are entered or if they are explicitly named in an <code>EVALUATE_FUNCTIONS</code> command. It is possible to enter a variable with a new expression any time. This expression is evaluated directly and its value stored as the value of the variable. Defined variables can be used as values in the <code>SET-CONDITION</code> command.• TABLES are used for listing results from the <code>STEP</code> or <code>MAP</code> commands. A table consists of a list of any number of state variables, functions or variables. Defined tables can also be used in the post-processor <code>POST</code>. <p> There is a special connection between tables and variables. If a variable is used in a table, it is evaluated for each line of the table in the <code>TABULATE</code> command or when the table is used in a plot.</p> |
| | <p>Name: <Name of the symbol></p> <p>Each symbol has a unique name that must start with a letter and can have maximum 8 characters.</p> <p>Legal characters include letters (either UPPER or lower case), digits and underscore <code>_</code>. Any other special character, such as parentheses (and), plus +, minus -, slash / or \, full stop (.), are illegal for symbol names.</p> <p>You can enter the symbol name and the value or function on the same line, these must be separated with an equal sign =, for example, <code>TC=T-273.15</code> or <code>T_C=T273.15</code> which stands for a definition of temperature in Celsius. Otherwise, these questions are asked.</p> |

| Syntax | ENTER_SYMBOL |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| |  <p>For different types of symbol (constant, function, variable or table), the questions have different prompts.</p> |
| | <p>Function: <Definition for a function or variable></p> <p><i>Functions</i> and <i>variables</i> are evaluated from an expression of state variables or other functions, constants or variables. The expression is a FORTRAN-like expression and operators +, -, *, = and ** can be used (** only with integer powers).</p> <p>Unary functions like LOG, LOG10, EXP, SIN, COS and ERF can also be used. An expression can be continued on more than one line. An expression should be terminated by a semicolon (;) or an empty line (by pressing <Enter> at the next prompt).</p> <p>Examples of function expressions:</p> <ul style="list-style-type: none"> • GM(LIQUID): The Gibbs energy of liquid per mole component • H.T/4.184: The heat capacity of the system in calories • ACR(CR)/X(FCC,CR): The activity coefficient for Cr in FCC • T-273.15: The temperature in Celsius <p>&: <Continuation of the definition for the symbol></p> <p>The ampersand & means that you can continue to write the function on the new line if one line is not enough for the function. If you finish the function press <Enter> again.</p> |
| | <p>Value: <Value for a constant></p> <p>A <i>constant</i> can only be assigned a numeric value once.</p> |
| | <p>Value or expression: <Value of expression for a variable></p> <p>A <i>variable</i> can be assigned a numeric value or an expression. An expression is evaluated immediately and discarded. Only the numeric value is kept. This gives a possibility to save a value between calculations with different conditions because all state variables and functions are evaluated for the new conditions.</p> |
| | <p>Variable(s): <Variable(s) in a table></p> <p>A <i>table</i> consists of a list of state variables or functions. One way to obtain results from a STEP command is through a table.</p> <p>Example:</p> <pre>ENTER TABLE K=T,X(LIQ,C),X(LIQ,CR),ACR(C)</pre> <p>Which means that the table called K contains four columns, i.e. the temperature, the mole fractions of C and Cr in the LIQUID phase, and the activity of C.</p> <p>To show the temperature in Celsius in a table, give the command ENTER_FUNCTION TC=T-273; and then use the symbol TC in the table.</p> <p>& <Continuation of the definition for the table></p> <p>The ampersand & means that you can continue to write the table on the new line if one line is not</p> |


| | |
|--------|--------------------------------------------------------------------|
| Syntax | ENTER_SYMBOL |
| | enough for the table. If you finish the table press <Enter> again. |

EVALUATE_FUNCTIONS



This command is available with the POLY and ED-EXP modules.

The value of one or more or all entered functions or variables are evaluated and listed.

| | |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | EVALUATE_FUNCTIONS |
| Prompt | <p>Name(s) : <Name(s) of defined function(s)></p> <p>The names of one or more entered functions or variables must be specified. By typing a wildcard *, all functions and variables are evaluated.</p> <p> Variables are evaluated only if these are explicitly named.</p> |

EXPERIMENT



This command is for the ED-EXP module.



This command is used in original experimental data files (*.POP or *.DOP), but can also be given interactively inside the ED-EXP module, to change the value or uncertainty of an experiment or to add more experimental information.



In the DICTRA module, you work with a .DOP file instead of a .POP file.

An experiment usually consists of two parts with a colon (:) separating them:

- as a quantity relation, and
- as the uncertainty of the value for the quantity,

The quantity relation can be a normal POLY module condition or an inequality (which is similar to condition but the relation between the quantity and given value is not in equality, i.e. < or >). The uncertainty can be expressed as an absolute value or relative to the value (x%).



An experiment that uses an inequality gives zero contribution to the sum of errors in the optimization procedure of PARROT if the value is on the right side. If the value is on the wrong side, the value after the colon determines how steeply the error increases with the value.

| Syntax | EXPERIMENT |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>The experiment must be typed after the command. Several experiments can be given on the same line.</p> <p>The syntax of EXPERIMENT is similar to a CONDITION. Usually, a state variable set equal to a value with a given uncertainty is specified after the colon (:). For example, <code>T=1273.15:5</code>.</p> <p>An inequality, <code><</code> or <code>></code>, can also be used. For example: <code>ACR(C)<-0.01:0.001, W(BCC,AG)>0.05:10%</code></p> |

ADDITIONAL INFORMATION ABOUT THE EXPERIMENT COMMAND

A typical experiment added interactively specifies that a phase should not be stable in a certain experiment, because a phase may appear in a range of composition or of temperature where it has never been observed during the optimization. A phase is unstable if its driving force is negative, and you can add experimental information to enforce that. For example, you can suppress the HCP phase in an existing experimental point:

```
CHANGE-STATUS HCP=DORMANT
EXPERIMENT DGM(HCP)<-.001:.0001
```



DGM is the POLY variable for the driving force that is already divided by RT , and it is dimensionless. Only dormant phases can have driving forces larger than zero, as this indicates that these would be stable if allowed to form. The experiment in the above case tries to modify the model parameters to make the HCP phase unstable.

More general examples of experiment definitions:

```
EXPERIMENT X(LIQ,PB)=.10:.01 X(FCC,PB)=0.02:.01
EXPERIMENT ACR(PB)=0.8:5%
EXPERIMENT T=700:5
```

The first experiment above describes a tie-line where the experimentally measured mole fraction of Pb is 0.1 in the liquid phase and 0.02 in the FCC phase, and its uncertainty is 0.01 for both measurements. The second experiment is that the activity of Pb should be 0.8 with an uncertainty of 5 percent.



The reference state of the component Pb must be set with the command SET_REFERENCE_STATE. The final one is that the temperature should be 700 K with an uncertainty of 5 degrees.

Experiments that are functions of states variable(s) must be described as the defined functions. For example:


```
ENTER_FUNCTION HTR=HM(LIQUID)-HM(FCC);
EXPERIMENT HTR=7000:1000
```

EXPORT



This command is for the ED-EXP module.

Transfer/export a calculated value from an equilibrium to an optimizing variable in the PARROT workspace. Thus the value can be used, for example, in the Gibbs energy description of a phase. This variable should not be optimized (i.e. it should be set as a fixed variable in PARROT).

| Syntax | EXPORT |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Function name: <Function name>#<n></p> <p>Specify the name of the function, the value of which should be transferred to a v variable. The number (n) of the v variable must be given after the function name, separated by hash character #.</p> <div>  <p>The function name is UPPER/lowercase sensitive, and it should normally be given in UPPER case.</p> </div> |
| | <p>EXAMPLE</p> <pre>Enter_function strngy=gm(fcc).x(cu); Export strngy#6</pre> <p>This transfers the value of the partial derivative of the Gibbs energy of the FCC phase with respect to the mole fraction of Cu to the optimizing variable 6 (i.e. v_6).</p> |

FLUSH_BUFFER



This command is for the ED-EXP module.

This command is only used in the *.POP file (i.e. it can also be used in the experimental data files). It is needed if the number of experiments require more space than can be fitted into one buffer.



In the DICTRA module, you work with a .DOP file instead of a .POP file.

When the PARROT program compiles experiments, it informs if any FLUSH commands are needed. FLUSH_BUFFER terminates the current block, saves it to the work file and starts a new block. With the READ command in the EDIT-EXP module, you can select the block to edit.

| Syntax | FLUSH_BUFFER |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | After a FLUSH_BUFFER command, the workspace is reinitiated and all functions or constants must be entered again in the *.POP file. You can take advantage of this; for example, you can use the FLUSH command to have blocks with different components in one *.POP file. |

GRAPHICS_PLOT



This command is for the ED-EXP module.

This command can help create a experimental data file from the *.POP file. Several data sets and different symbols are allowed.



In the DICTRA module, you work with a .DOP file instead of a .POP file.

| Syntax | GRAPHICS_PLOT |
|--------|-----------------------------------------------|
| | <Dataset#> <X value> <Y value> <Symbol index> |

IMPORT



This command is for the ED-EXP module.

Transfer/import the value of one of the optimizing variables to a constant. Normally, it is directly used inside an experimental data (*.POP) file. It is the opposite of the EXPORT command.




In the DICTRA module, you work with a .DOP file instead of a .POP file.

The IMPORT command is useful if several experiments are done at the same activity of a component, but this activity is not known. The activity should then be optimized and all equilibria with the same activity should use the same value. In this case the variable must be set as an optimizing variable, and an initial guess of the activity should be given. During the optimization, the PARROT program tries to find the activity that gives the best fit.



If an approximate value of the activity is known, it can be supplied as an experiment.

| Syntax | IMPORT |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Constant name: <Constant name>#<n></p> <p>The value of the v variable must be assigned a symbolic constant. The number (n) of the v variable must be given after the constant name, separated by hash character #.</p> <div>  <p>The constant name is UPPER/lowercase sensitive, and it should normally be given in UPPER case.</p> </div> |
| | <p>EXAMPLE</p> <p>Enter_constant acu=0.1</p> <p>Import acu#2</p> <p>This transfers the value of the optimizing variable 2 (i.e. v_2) to the constant ACU.</p> |

LABEL_DATA



This command is for the ED-EXP module.

Add a label to the experimental equilibrium point, either as a single point or several points given individually or in a table. The label is maximum four characters and must start with the letter A. Normally, it is directly used inside an experimental data file (*.POP).



In the DICTRA module, you work with a .DOP file instead of a .POP file.

Several experimental equilibria can be given the same label, and the label can be used with SET_WEIGHT to assign the same weight to all equilibria with the same label.

| Syntax | LABEL_DATA |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Label? /A1/: a<bcd></p> <p>Specify a textual label (as maximum characters and must start with the letter A) for the current experimental equilibrium point(s).</p> |

LIST_ALL_EQUILIBRIA



This command is for the ED-EXP module.

| Syntax | LIST_ALL_EQUILIBRIA |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>List all the details (including equilibrium indicators, labels, iteration numbers, weight, and fixed phases or comments) of all equilibrium points from the current one to the last one on screen. You</p> |

| | |
|--------|----------------------------------------------------------------------------------------------------------------|
| Syntax | LIST_ALL_EQUILIBRIA |
| | can always use SELECT_EQUILIBRIUM to select a specific point as the current equilibrium point for such a list. |

LIST_CONDITIONS



This command is available with the POLY and ED-EXP modules.

All the conditions that are set by the SET_CONDITION command and the command-sequence CHANGE_STATUS PHASE =FIXED <0 or 1 or alike>, are listed. The current conditions are also listed by the LIST_EQUILIBRIUM command. The degree of freedom in the defined system is also shown.

- If this is zero, you can perform a COMPUTE_EQUILIBRIUM command.
- If it is larger than zero, some more conditions are required, and you must further set additional ones, using SET_CONDITION or CHANGE_STATUS.
- If it is negative, then too many conditions are defined and the unnecessary ones conditions need to be removed using the SET_CONDITION command (with a value of NONE for the to-be-deleted condition) or the CHANGE_STATUS command (i.e. changing a FIXED status of a phase to another type of phase status, ENTERED or DORMANT or SUSPENDED).

| | |
|---------|------------------------------------------------------------------------------------------------|
| Syntax | LIST_CONDITIONS |
| Example | <pre>P=100000, T=800, N(NI)=1E-1, N=1 FIXED PHASES FCC_A1=1 LIQUID=0 DEGREE OF FREEDOM 0</pre> |

LIST_EQUILIBRIUM




This command is available with the POLY and ED-EXP modules.

The result (always in SI units) from the last calculated equilibrium is listed on screen or in a text file.



You can also execute this command if no calculation is made or if the calculation fails. Make sure to interpret the results accordingly.

| | |
|--------|------------------------------------------------|
| Syntax | LIST_EQUILIBRIUM |
| Prompt | Output to screen or file /Screen/: <File name> |

| Syntax | LIST_EQUILIBRIUM |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | The name of the text file where the list of the calculation results shall be written. |
| | Options /VWCS/: <Option(s)> Select the output units and formats by optionally specifying a combination of these letters. <ul style="list-style-type: none"> • <i>Fraction order</i>: V means VALUE ORDER; A means ALPHABETICAL ORDER. • <i>Fraction type</i>: W means MASS FRACTION; X means MOLE FRACTION. • <i>Composition</i>: C means only COMPOSITION; N means CONSTITUTION and COMPOSITION. • <i>Phase</i>: S means including only STABLE PHASES; P means including ALL NON-SUSPENDED PHASES. |
| | <p>Default options are VWCS. If the output fraction type should be in mole fraction (rather than mass fraction), then give VXCS or type X (implying that in this case the options V, C and S are accepted as the listing manners for fraction order, composition and phase).</p> <p>If accepting all the default options, or if accepting all the altered options that had already changed when using this command previously, you can type L_E,,, or LIST_EQUILIBRIUM ,,,</p> <p> LIST_EQUILIBRIUM displays ORD (ordered) or DISORD (disordered) (when available). See "CHANGE_LEGEND" on page 354 for details.</p> |

LIST_STATUS




This command is for the ED-EXP module.



There is also a POLY module command with the same name.

List the status of components, species or phases.

| Syntax | LIST_STATUS |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Specify what to list:</p> <p>Option /CPS/:<keyword(s)></p> <p>keyword = C or P or S, or any combination</p> <ul style="list-style-type: none"> • C: list component status • P: list phase status • S: list species status • CS: list both components and species <p>Default is CPS.</p> |
| | The results depend on the key word specified in the options for CHANGE_STATUS , a table with the |

| Syntax | LIST_STATUS |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>current status of phases or species or components, or the combinations, is shown:</p> <ul style="list-style-type: none"> • For components, the statuses and reference states are listed. • For species, only the status is listed. • For ENTERED and FIXED phases, the status, driving forces and equilibrium amounts are listed. |
| | <div>  <p>The metastable phases are listed in descending order of stability. To avoid long outputs only 10 metastable phases (in ENTERED status) are listed by lines, while all other less stable phases are merged onto one line. For DORMANT phases, their phase names and driving forces are listed. For SUSPENDED phases, only the phase names are listed.</p> </div> |

LIST_SYMBOLS



This command is for the ED-EXP module.



There are also POLY and POST module commands with the same name.

Use this command to list the definitions for all constants, functions, variables and tables. In order to find the value of a function or variable, use SHOW_VALUE or EVALUATE_FUNCTIONS. A table is tabulated with the TABULATE command.

| Syntax | LIST_SYMBOLS |
|--------|----------------------------------------------------------------------------------------------------------------------------------|
| | The defined variables are listed up together with the defined functions, but variable names are followed by a percentage sign %. |

MAKE_POP_FILE



This command is for the ED-EXP module.



In the DICTRA module, you work with a .DOP file instead of a .POP file.

Use this command to make interactive changes and additions to the original experimental data file (the *.POP or *.DOP file). For example, to document or transfer the current or final experimental data to a *.POP file, this command will write it to a new *.POP file or overwrite previous versions.




Check the output carefully for errors. Tables in original *.POP files are written as individual experimental points. The output can be shown on screen or be saved as a new *.POP file where to write or overwrite the edited experimental information in a simple text format.

| Syntax | MAKE_POP_FILE |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | Output to screen or file /Screen/: <POP/DOP-file name> Specify a name of the new *.POP file where to write or overwrite the edited experimental information in a simple text format. If an existing *.POP file name is specified, it is overwritten. |

READ_WORKSPACES



This command must be given each time the ED_EXP module is entered, unless it is already given once in ED_EXP and does not use LIST_RESULT or OPTIMIZE_VARIABLES in PARROT in between.

| Syntax | READ_WORKSPACES |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | Block number /#/: <n> The number of a data block that should be edited must be given. If there is no FLUSH_BUFFER command in the original POP file, then there is only one data block with the number 1. |
| |  READ_WORKSPACE = READ This command is equivalent to READ_WORKSPACES in the POLY module, but it only reads the POLY workspace from the work file set by SET_STORE_FILE in the PARROT module. |

REINITIATE_MODULE



This command is for the ED-EXP module.

The REINITIATE_MODULE command makes sure that the entire ED-EXP module is reinitiated to the original state.

| Syntax | REINITIATE_MODULE |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | All the defined components, defined conditions, changed status, entered symbols, defined independent axis-variables, calculated starting equilibrium-points, added initial equilibrium points, stepped/mapped equilibrium data, and so forth, are removed completely. The saved file name is |

| | |
|--------|-------------------|
| Syntax | REINITIATE_MODULE |
|--------|-------------------|

| | |
|--|--------------------------|
| | restored to the default. |
|--|--------------------------|

RESTORE_ALL_WEIGHTS



This command is for the ED-EXP module.

Restore a specific weight-set (previously saved by STORE_ALL_WEIGHTS) and assign all the different experimental points in the current data block with the previously-set weights in the sequential assessments.

| | |
|--------|---------------------|
| Syntax | RESTORE_ALL_WEIGHTS |
|--------|---------------------|

| | |
|--------|--------------------------------------------------|
| Prompt | Set number (0 for list) /0/: <weight-set number> |
|--------|--------------------------------------------------|

| | |
|--|----------------------------------------------|
| | The default value 0 is for a list on screen. |
|--|----------------------------------------------|

SAVE_WORKSPACES



This command is for the ED-EXP module.

In the PARROT workspace this command saves the current status of the ED_EXP submodule before you switch back to the PARROT module. This is required when you want to save equilibria changes, including changes to conditions, experimental data, and/or computed equilibria results, as well as any newly added equilibria.


With this command all the changes made in the ED_EXP submodule are saved in the PARROT workspace. This means you do not need to execute SAVE_PARROT_WORKSPACES in the PARROT module.

However, when in the PARROT module, additional changes can only be saved with the SAVE_PARROT_WORKSPACES command even if they have been made prior to executing SAVE_WORKSPACES in ED_EXP.

When you exit the ED_EXP (or Thermo-Calc), the next time the file is opened it is in the same state as when you executed the SAVE_WORKSPACES command. However, if you use OPTIMIZE_VARIABLES the computed results are automatically updated.

| | |
|--------|-----------------|
| Syntax | SAVE_WORKSPACES |
|--------|-----------------|

| | |
|--------|-------------|
| Prompt | <File name> |
|--------|-------------|

| Syntax | SAVE_WORKSPACES |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| |  Sometimes good starting values (SET_START_VALUE) are required to successfully get or compute an equilibrium correctly. In this case, it is important to save the computed equilibrium in the PARROT workspace. It is important to remember that the computed results can be ruined by improper optimizations. For this reason, it is suggested you save the .PAR file with a different name to back up the PARROT workspace. |

SELECT_EQUILIBRIUM



This command is available with the POLY and ED-EXP modules.

If you create more than one initial equilibrium (during data-assessments using the PARROT/ED_EXP modules), you can switch between them using this command.

| Syntax | SELECT_EQUILIBRIUM |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Number /Next/: <Choice on equilibrium></p> <p>Options: FIRST, LAST, NEXT, PREVIOUS or PRESENT.</p> <p>Most commands affect only the PRESENT equilibrium. However, the REINITIATE_MODULE and DEFINE_COMPONENTS commands remove all the stored equilibria.</p> |


SET_ALL_START_VALUES



This command is available for the POLY and ED-EXP modules.

Set start values, e.g. if the calculation fails or if you have a miscibility gap or ordering. If temperature and pressure are not conditions, you are asked for values of them. Then for each phase prompt on if it should be stable and on its constitution.

| Syntax | SET_ALL_START_VALUES |
|---------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>T /XXXX/: <Temperature in K></p> <p>If the temperature is not a condition, supply a guess of its final value (in K).</p> |
| | <p>P /100000/: <Pressure in Pa></p> <p>If the pressure is not a condition supply a guess of its final value (in Pa).</p> |
| Prompts | <p>Automatic start values for phase constitutions? /N/: <Y, N or F></p> <ul style="list-style-type: none"> For N, enter an initial amount of each entered phase and the major constituents or site fraction of each constituent. For Y, the program automatically sets the start values for phase constitutions in all possible phases. |

| Syntax | SET_ALL_START_VALUES |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <ul style="list-style-type: none"> • F is for force. In some cases the calculation fails because impossible conditions are set, e.g. $w(C)=1.5$ ($w(C)$ is mass fraction and must thus be less than unity. The program tries to fulfill this condition by putting maximum amount of carbon in all phases, but can fail anyway. When you detect the error and set $w(C)$ to 0.015, the calculation may still fail because it could start from the previous values. To get back to 'fresh' start values, choose F. |
| | <p>Should <phase> be stable /N/: <Y/1 or N/2></p> <p>A guess if this phase should be stable or not is requested. All entered phases are prompted for this question and next two.</p> <div style="border: 1px solid black; padding: 10px; margin: 10px 0;">  <p>You cannot have more phases stable than you have components, but at least one (which dissolves all constituents) must be set as stable. For backward compatibility, this question can be answered by 1 (for Yes) or 0 (for No).</p> </div> <p>The phase name may have a hash sign # followed by a digit, e.g. BCC_A2#2. For phases with miscibility gaps, there should be two phases with the same name but with different numbers after the hash sign.</p> |
| | <p>Major constituent(s): <Name of major constituent(s) in the phase></p> <p>The constituent with the largest fraction in the phase should be specified. If there are more than one constituent with a large fraction, give them all on the same line. If the default major constituents should be used answer with an asterisk (*). By giving \$ the constitution is not changed. If there should be no major constituent give NONE and or if the major constituent(s) are improperly specified, you are asked for individual fractions in the phase.</p> |
| | <p>Y(<phase>,<constituent>) /.XXXXXXXXXX/: <.YYYYY></p> <p>The current value (.XXXXXXXXXX) is default. You can accept the default by pressing <Enter> or give a new value (.YYYYY).</p> <p>The phase name or constituent name may have a hash sign # followed by a digit, e.g. Y(BCC_A2#2,FE), Y(BCC_A2#2,C#2). For phases with miscibility gaps, there should be two phases with the same name but with different numbers after the hash sign. For phases with sublattices, the constituents in sublattice 2 or higher is also be suffixed with a hash sign # followed by a digit.</p> |

SET_ALTERNATE_CONDITION



This command is for the ED-EXP module.



A special command used in the experimental data *.POP file but also possible in the ED_EXP module. It is used only when you have specified that the alternate mode is set in the PARROT module.



In the DICTRA module, you work with a .DOP file instead of a .POP file.


The command syntax is almost the same as for the POLY command SET_CONDITION while the uncertainty should also be specified.



The alternate condition (including the normally POLY module condition plus uncertainty; see below) must be given explicitly, but can be given on the same line or on separate lines with each one started with the command.

| Syntax | SET_ALTERNATE_CONDITION |
|--------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | State variable expression: <State variable name or linear expression> Give either a state variable or a linear expression of state variables. |
| Options | Description and Information |
| State variables | <p>Some of the state variables that can be used in conditions are:</p> <ul style="list-style-type: none">• T: temperature in the system (in K)• P: pressure in the system (in Pascal)• N: system size (mole number in moles)• B: system size (mass in grams)• N(<component>): mole number of a component in the system• X(<component>): mole fraction of a component in the system• W(<component>): weight fraction of a component in the system• For the SET_CONDITION command this is ACR(<component>): activity of a component in the system. For the SET-ALTERNATIVE_CONDITION command, this is ACR(<phase>,<component>) (activity of a component in a phase)• For the SET_CONDITION command this is MUR(<component>): chemical potential of a component in the system. For the SET-ALTERNATIVE_CONDITION command, this is MUR(<phase>,<component>) (chemical potential of a component in a phase)• X(<phase>,<component>): mole fraction of a component in a phase• W(<phase>,<component>): weight fraction of a component in a phase• ACR(<species>,<phase>): activity of a species in a solution phase• MUR(<species>,<phase>): chemical potential of a species in a solution phase• H: enthalpy in the system (in J)• HM(<phase>): enthalpy of a phase (in J/mol) |
| Additional prompts | <p>Factor: <A factor for the state variable, or a continuation></p> <p>This question means that the previous question was not answered. The program is then expecting a single state variable or a complete state variable expression, or the numeric factor in an expression with only one state variable. In a state variable expression a state variable may be preceded by a constant factor. An example of this is:</p> |

| Syntax | SET_ALTERNATE_CONDITION |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <pre>2*MUR (FE) +3*MUR (O) =-35000</pre> <p>This means that it should be a condition that two times the chemical potential of FE plus three times the chemical potential of O should be -35000 J/mol.</p> |
| | <p>State variable: <A specified state variable, or a continuation></p> <p>This question is prompted if a single state variable name has not given in either the prompt <code>State variable expression</code> or <code>Factor</code>, or a state variable expression is given but the expression is incomplete, for example, <code>T-</code> or <code>2*MUR (FE) +</code>, for which the program is then expecting a continuation of the unfinished expression. You need to specify a state variable or a complete state variable expression, or complete the unfinished state variable expression. If a numeric factor is given before this prompt, only one state variable can be specified; otherwise, the program only takes the first state variable to complete the expression (i.e. the factor times the state variable).</p> |
| | <p>Value /X/: <A numeric value, a constant or a variable></p> <p>The value of the condition. This can be a numeric value, a constant or a variable. A suggestion is given as the default value. The special value <code>NONE</code> means that the condition is removed.</p> |
| | <p>Uncertainty /None/: <Uncertainty of the condition></p> <p>The uncertainty of the condition. This can be a numeric value, a constant or a variable. The default value <code>NONE</code> means that the uncertainty for the value specified above is zero. The uncertainty can either be expressed as an absolute value or relative to the value of the condition in percent (%).</p> |
| Notes | <p>There are more state variables that can be used in conditions. For more information, type an <code>INFO STATE_VARIABLES</code> command in the POLY module. A condition is normally a value of a single state variable with its value.</p> <p>FOR EXAMPLE:</p> <pre>T=1273.15 P=1E5 X (C) =.002 W (CR) =1.5 ACR (CR) =0.85 X (FCC, C) =.001 H=-250000 HM (BCC) =-225000</pre> <p>A condition can also be a value of a linear expression involving more than one state variable.</p> <p>FOR EXAMPLE:</p> <pre>X (LIQ, S) -X (PYRR, S) =0</pre> <p>This means that it is a condition that the mole fraction of <code>s</code> should be the same in the LIQUID and PYRRHOTITE phases. In practice that should be the congruent melting point.</p> |

| | |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | SET_ALTERNATE_CONDITION |
| |  After the equal sign only a numeric value is allowed. |


SET_CONDITION



This command is available with the POLY and ED-EXP modules.

Specify the equilibrium conditions for the calculation. All kinds of state variables, as well as most of the $M/W/V/F$ -suffixed state variables (for normalization) and R -suffixed state variables (with respect to chosen reference states), can be used as conditions. In addition to temperature and pressure conditions, a multicomponent system can have mixed types of conditions. You should repeat this command for a multicomponent system until the degree of freedom in the defined system becomes zero. When a **FIXED** phase status is used on a specific phase (use **CHANGE_STATUS**), it is equivalent to one condition (implying that particular phase is stable in the defined system).

| | |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | SET_CONDITION |
| | <p>Each condition must be given explicitly, but can be given on the same line (separated by a comma (,) or an empty space) or on separate lines with each one started with the command.</p> <p>EXAMPLE</p> <pre>SET_COND T=1273, P=1E5, W(C)=.0015, X(LIQ,CR)=.22, ACR(N)=.2</pre> <p>or</p> <pre>SET_COND T=1273, P=1E5 SET_COND W(C)=.0015, X(LIQ,CR)=.22 ACR(N)=.2</pre> <p>In this example, the temperature is set to 1273 K, the pressure to 1 bar (1E5 Pascal), the mass (weight) fraction of C to 0.0015 and the mole fraction of Cr to 0.22 and the activity of N to 0.2.</p> |
| Prompt | <p>State variable expression: <State variable name or linear expression> or a linear expression of state variables.</p> <p>Some of the state variables that can be used in conditions are:</p> <ul style="list-style-type: none"> • T: temperature in the system (in K) • P: pressure in the system (in Pascal) • N: system size (mole number in moles) • B: system size (mass in grams) • N(<component>): mole number of a component in the system • X(<component>): mole fraction of a component in the system • W(<component>): weight fraction of a component in the system • For the SET_CONDITION command this is ACR(<component>): activity of a component in the |

| Syntax | SET_CONDITION |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>system. For the SET-ALTERNATIVE_CONDITION command, this is <code>ACR(<phase>,<component>)</code> (activity of a component in a phase)</p> <ul style="list-style-type: none"> • For the SET_CONDITION command this is <code>MUR(<component>)</code>: chemical potential of a component in the system. For the SET-ALTERNATIVE_CONDITION command, this is <code>MUR(<phase>,<component>)</code> (chemical potential of a component in a phase) • <code>X(<phase>,<component>)</code>: mole fraction of a component in a phase • <code>W(<phase>,<component>)</code>: weight fraction of a component in a phase • <code>ACR(<species>,<phase>)</code>: activity of a species in a solution phase • <code>MUR(<species>,<phase>)</code>: chemical potential of a species in a solution phase • <code>H</code>: enthalpy in the system (in J) • <code>HM(<phase>)</code>: enthalpy of a phase (in J/mol) <p>There are many state variables that can be used in conditions. For more information, enter an <code>INFO STATE_VARIABLES</code> command. A condition is normally a value of a single state variable with its value.</p> <p>EXAMPLE</p> <pre>T=1273.15 P=1E5 X(C)=.002 W(CR)=0.5 ACR(CR)=0.85 X(FCC,C)=.001 H=-250000 HM(BCC)=-225000</pre> <p>A condition can also be a value of a linear expression involving more than one state variable. For example,</p> <pre>X(LIQ,S)-X(PYRR,S)=0</pre> <p>This means that it is a condition that the mole fraction of <code>s</code> component should be the same in the LIQUID and PYRRHOTITE phases. In practice, that should be the congruent melting point.</p> <div>  <p>After the equal sign only a numeric value is allowed in the expression.</p> </div> <p>Factor: <A factor for the state variable, or a continuation></p> <p>This question means you did not answer the previous question. The program is then expecting a single state variable or a complete state variable expression, or the numeric factor in an expression with only one state variable. In a state variable expression a state variable may be preceded by a constant factor. An example of this is:</p> <pre>2*MUR(Fe)+3*MUR(O)=-35000</pre> <p>This means that it should be a condition that two times the chemical potential of <code>Fe</code> plus three times the chemical potential of <code>O</code> should be -35000 J/mol.</p> |

| Syntax | SET_CONDITION |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>State variable: <A specified state variable, or a continuation></p> <p>This question is prompted if a single state variable name has not given in either the prompt <code>State variable expression</code> or <code>Factor</code>, or a state variable expression is given but the expression is incomplete, for example, <code>T-</code> or <code>2*MUR(Fe)+</code>, for which the program is then expecting a continuation of the unfinished expression. You need to specify a state variable or a complete state variable expression, or complete the unfinished state variable expression. If a numeric factor is given before this prompt, only one state variable can be specified; otherwise, the program only takes the first state variable to complete the expression (i.e. the factor times the state variable).</p> |
| | <p>Value /X/: <A numeric value, a constant or a variable></p> <p>The value of the condition. This can be a numeric value, a constant or a variable. A suggestion is given as the default value. The special value <code>NONE</code> means that the condition is removed; for example <code>T=NONE</code> takes away the temperature condition.</p> |

SET_NUMERICAL_LIMITS



This command is available for the POLY, Scheil and ED-EXP modules.


Change the criteria for convergence. This is to speed up a calculation in a complex system.

If there is any convergence problem in finding a stable solution at any stage during a calculation procedure enforced by `COMPUTE_EQUILIBRIUM`, `STEP_WITH_OPTIONS`, `MAP` or `ADVANCED_OPTIONS`), this message displays:

```
Convergence problems, increasing smallest site-fraction from
1.00E-30 to hardware precision 2.00E-14. You can restore using
SET-NUMERICAL-LIMITS
```

This implies that smallest site fraction in the current POLY workspace is automatically increased from the default value `1.00E-30` to the hardware-dependent precision (under Linux, as `2.00E-14`). For other subsequent POLY module calculations, you can use this command to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

| Syntax | SET_NUMERICAL_LIMITS |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Maximum number of iterations /500/:</p> <p>By default, the program tries 500 iterations before it gives up. As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.</p> |
| | <p>Required accuracy /1E-6/:</p> <p>This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.</p> |

| Syntax | SET_NUMERICAL_LIMITS |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>Smallest fraction /1E-12/:</p> <p>This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions.</p> <p>The default value for the smallest site-fractions is 1E-12 for all phases, except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as 1E-30 (unless you have used the SET_NUMERICAL_LIMITS command to reset an even-lower value (e.g. 1E-45, that is naturally enforced to all the phases in the system).</p> |
| | <p>Approximate driving force calculation for metastable phases /Y/:</p> <p>Normally the POLY module only requires that the set of stable phases is in equilibrium in order to terminate the iterations. By default, the metastable phases are included in all iterations but these may not have reached their most favourable composition and thus their driving forces may be only approximate.</p> <div>  <p>If it is important that these driving forces are correct, choose N to force the calculation to converge for the metastable phases. This may require more iterations, and the STEP and MAP command may also terminate due to bad convergence in a metastable phase.</p> </div> |

SET_REFERENCE_STATE



This command is available for the POLY, ED-EXP and POST modules.

The reference state for a component is important when calculating activities, chemical potentials and enthalpies and is determined by the database being used. For each component the data must be referred to a selected phase, temperature and pressure, i.e. the reference state.





All data in all phases where this component dissolves must use the same reference state. However, different databases can use different reference states for the same element/component. It is important to be careful when combining data obtained from different databases.

By default, activities, chemical potentials and so forth are computed relative to the reference state used by the database. If the reference state in the database is not suitable for your purposes, use this command to set the reference state for a component using `SER`, i.e. the Stable Element Reference (which is usually set as default for a major component in alloys dominated by the component). In such cases, the temperature and pressure for the reference state is not needed.

In order to specify conditions in the specific reference state, you can append an R to the state variables. Thus, AC is the activity (of a system component or of a species in a phase) with respect to the default reference state, and ACR is the activity with respect to the selected reference state; MU is the chemical potential of a system component with respect to the default reference state, and MUR stands for the chemical potential with respect to the selected reference state. The AC and ACR variables, for both components in a system and species in a phase, can be specified in natural logarithm, e.g. $LNAC(Fe)$, $LNACR(C)$, $LNAC(O_2,GAS)$, $LNACR(O_2,GAS)$.

For the POST module, and after calculating with the `STEP_WITH_OPTIONS` or `MAP` commands, the reference state for a component can also be changed to plot various properties of the component in the entire system or in a specific phase. Then you can set the diagram axes as the chemical potential or activity quantities with the R suffix, i.e. $MUR(comp)$, $MUR(comp,ph)$, $ACR(comp)$, $ACR(comp,ph)$ or the common logarithms [e.g. $LNACR(comp,ph)$].

| Syntax | SET_REFERENCE_STATE |
|---------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Component: <Name of the component></p> <p>The name of the component must be given.</p> |
| | <p>Reference phase: <Name of a phase used as the new reference state></p> <p>Enter the Name of a phase for the system.</p> <div>  <p>For a phase to be usable as a reference for a component, the component needs to have the same composition as an end member of the phase. The reference state is an end member of a phase. The selection of the end member associated with the reference state is only performed once this command is executed.</p> </div> <p>If a component has the same composition as several end members of the chosen reference phase, then the end member that is selected at the specified temperature and pressure will have the lowest Gibbs energy.</p> <p>The following are example using temperature. Pressure is used in the same way:</p> <ul style="list-style-type: none"> • In the Fe-C system, BCC can be a reference state for Fe but not for C since BCC can exist as pure Fe but cannot exist as pure C. • If GAS is chosen as the reference phase of component O at such a high temperature that O1 has the lowest energy, then O1 remains the reference state even at calculations performed at lower temperatures where O2 has a lower energy than O1. • Setting the reference state for component O as gas (one sublattice) with constituents O1, O2 and O3 results in O2 being the reference state if, at the present temperature, pure O2 has the lowest energy of O1, O2 and O3. If the reference state is set above a critical higher temperature, then O1 has the lowest energy and consequently becomes the reference state. |
| | <p>Temperature /*/: <Temperature for the reference state></p> <p>Select the Temperature (in K) for the reference state. The wildcard value * means the current temperature is used at the time of evaluation of the reference energy for the calculation.</p> |

| Syntax | SET_REFERENCE_STATE |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| |  The temperature set with this command does not affect the temperature used when evaluating the energy of the reference state during the end member selection process. |
| | <pre>Pressure /1E5/: <Pressure for the reference state></pre> <p>Select the Pressure (in Pa) for the reference state. The wildcard value * means the current pressure is used for evaluating the reference energy at the time of calculation.</p> |
| | <p>EXAMPLES</p> <pre>S-R-S Fe SER S-R-S Cr FCC * 100000 S-R-S H2O AQUEOUS * 100000 S-R-S ZE REF_ELECTRODE * 100000</pre> |

SET_START_CONSTITUTION



This command is available with the POLY and ED-EXP modules.

This command is similar to SET_ALL_START_VALUES, but is used for an individual phase that may have a wrong constitution.

| Syntax | SET_START_CONSTITUTION |
|---------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Phase name: <Name of a phase, and possible major constituent(s)></p> <p>Specify the name of a phase for which the constitution shall be set.</p> <p>If there is a major constituent of the phase, you must specify this on the same line as the phase name. By giving an*, select the default major constituents. A \$ means keeping the same constitution, and NONE means to give individual site-fractions.</p> |
| | <pre>Y(<Phase>#<Composition_set>,<Constituent>#<Sublattice>) /xxx/: <SF></pre> <p>The site fraction ($_{SF}$) of the constituent shall be given. The default value xxx is the last calculated one.</p> |

SET_START_VALUE



This command is available with the POLY and ED-EXP modules.



This command is not often required as the automatic start values can be handled for most problems.

Set a start value of an individual variable.

| Syntax | SET_START_VALUE |
|---------|---------------------------------------------------------------------------------|
| Prompts | State variable: <Name of a state variable> The state variable must be given. |
| | Value Specify the value to be assigned the state variable as start value. |

SET_WEIGHT



This command is for the ED-EXP module.




Each experimental value has an uncertainty associated with it, specified by the value after the colon (:) with the command EXPERIMENT. During an optimization the absolute difference between the experimental and calculated values gives a contribution to the sum of error.

With the SET_WEIGHT command, you can change the scale of such a contribution (the uncertainty) for a single experimental point, or the contributions (all uncertainties) for a set of equilibria. The default weight is always unity. A value smaller than one means that the experiments should have less weight. A value larger than one that these should have higher weight. The special value zero means that the set of equilibria should be ignored in editing in ED_EXP (as is given) and in OPTIMIZE_VARIABLES in PARROT.



The weight may be needed to obtain a balance between different kinds of experiments. For example, if there are only five experimental values of the composition of a phase diagram but 500 experimental values of activities or enthalpies, then the five composition points may have to be given higher weight than unity, otherwise these are not well described by the optimizing procedure.

| Syntax | SET_WEIGHT |
|---------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | Value /1/: <Weight value> Specify a weight of the experiments in the specified equilibria (asked in the next prompt). The contribution to the sum of errors of these experiments are multiplied by this weight. |


| Syntax | SET_WEIGHT |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| |  The weight is squared, thus use 0.7 to make the error half (0.49) as big, and 1.4 to make it twice (1.96) as large. |
| | <p>Equilibria (range) or label(s) /Present/:<Selection></p> <p>Define the equilibria. These are available in the read data block from the current work file and are given the above-defined weight.</p> <p>The selection may be given as a range but the equilibrium numbers must then be separated only by a minus sign.</p>  The start and end equilibrium numbers must be available in the read data block read from the current work file. <p>For example, 5-101, means that all equilibria starting from the identifier 5 until the identifier 101. Some of numbers between these two identifiers may not exist in the data block.</p> <p>The selection may also be given as one or more labels (which should be separated only by a space). All equilibria with the specified label(s) in the read data block are given the above-defined weight.</p> <p>By pressing <Enter> to accept the default value <code>present</code>, the above defined weight is only assigned to the current or present experimental point (which is selected by the POLY SELECT_EQUILIBRIUM command).</p>  If is used but no specific equilibrium point is selected afterwards, the last point in the read data block remains the <code>present</code> point. |


SHOW_VALUE



This command is available for the POLY and ED-EXP modules.

Show the current value of any state variable, function or variable.

| Syntax | SHOW_VALUE |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>State variable or symbol: <Name(s) of state variable(s) or symbol(s)></p> <p>A single or several state variables or symbols (entered functions or variables) can be specified.</p> |
| |  The wildcard * can be used to denote all phases or all components. <p>You can use the dollar-sign \$ to denote all stable phases. Thus, the command SHOW W(*,*)lists the mass fraction of all phases, whereas SHOW W(\$, *) lists the mass fraction of all stable phases.</p> |

| Syntax | SHOW_VALUE |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| |  <p>If you <code>SHOW</code> a function, all functions are evaluated using the current values of the state variables. But if you <code>SHOW</code> a variable, it retains its value from the time it was <code>ENTERED</code> or last <code>EVALUATED</code>.</p> <p>Therefore to save a value from one calculation to another, <code>ENTER</code> it to a variable. This is frequently done in the PARROT module to transfer values between equilibria.</p> |

STORE_ALL_WEIGHTS

Store a new weight-set that is the current situation of specified weights for all the different experimental points read from the currently-selected experimental data block in an assessment. This is useful when you want to try various weight-settings for some experimental points or for all the points, and then compare the assessment results from different weight-sets. Such a saved weight-set can be recalled and restored for all experimental data point with `RESTORE_ALL_WEIGHTS` sequentially.

| Syntax | STORE_ALL_WEIGHTS |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Command line: <Weight-set name></p> <p>Give a weight-set name (comment line texts) for the current weight set for all experimental points.</p> |

TABLE_HEAD, TABLE_VALUES and TABLE_END

These commands are used only in the *.POP file. It represents a convenient way to enter many experimental measurements of the same type in a table format.



In the DICTRA module, you work with a .DOP file instead of a .POP file.



These commands should always be used together and in a sequence, meaning that a table should always start with the `TABLE-HEAD` command, then `TABLE-VALUES`, and finish with `TABLE-END`. Between `TABLE_HEAD` and `TABLE-VALUES` also add definition lines (e.g. on phase status, reference states, conditions, experiments, labels, etc.) for the experimental measurements of the current information type.

| | |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | TABLE_HEAD TABLE_VALUES TABLE_END |
| Prompt | |
| | <p>After the TABLE-HEAD command, there must be an equilibrium description similar to a single experimental equilibrium but with some special notation. Then, there is always a TABLE-VALUES command, after which the actual data is given in columns. At the end of each table, there must be a TABLE-END command.</p> <p>The TABLE-HEAD command must be followed by a numeric value. This is used to generate unique numeric identifiers for all the equilibria in the table. The numeric identifier is incremented by one for each experimental (equilibrium) point in the table.</p> |
| | <p>EXAMPLE</p> <p>An example of the use of a table for enthalpy measurements in the liquid is given here. Much more elaborate tables can be used</p> <pre> \$ Enthalpies of mixing, Topor and Kleppa, Met Trans 1984 TABLE-HEAD 1 CREATE-NEW @@ 1 CHANGE-STATUS PHASE LIQ=FIX 1 SET-REFERENCE-STATE AU LIQ * 1E5 SET-REFERENCE-STATE CU LIQ * 1E5 SET-CONDITION P=1E5 T=1379 X(LIQ,AU)=@1 LABEL ALH EXPER HMR=@2:5% TABLE-VALUES 0.0115 -322 0.0563 -1520 0.8499 -2976 0.9002 -2114 TABLE-END </pre> |
| | <p>The equilibrium description between TABLE-HEAD and TABLE-VALUES is similar as for a single experiment, except for these details:</p> <ul style="list-style-type: none"> • @@ Used to automatically generate a series of identifying numbers instead of creating only one with the command CREATE_NEW_EQUILIBRIUM. The program automatically generates the identifying numbers starting after the number given after the TABLE-HEAD command (in this case it is 1). • @1 values in the table are specified by an @ sign followed by a column number. In the above case, the mole fraction of Au in the liquid is in column 1 (see the line for SET_CONDITION). The columns may have other information than values, and you can use phase names or any text. If the text contains spaces or special characters, it must be surrounded by double quotes in the table, e.g. "ABC DEF&ghi". • For the <i>syntax checker</i> all commands describing the equilibrium must be in UPPER case after |

| | |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | TABLE_HEAD TABLE_VALUES TABLE_END |
| | <p>the TABLE_HEAD command.</p> <ul style="list-style-type: none"> After the TABLE-VALUES command, there should be one line for each experimental measurement of the same type giving the values or texts that should be copied into the places of the condition or experiment defined by @1, t, etc. You can have columns that are not used but there must be exactly the same number of columns of each line, otherwise the syntax checker gives an error message in the PARROT module. |

TRANSFER_START_VALUES



This command is for the ED-EXP module.

In the ED_EXP module it is time consuming to calculate all equilibria when the optimization is sensitive to start values of the composition of the phases. Usually in one data block there are several experimental points with the same kind of equilibrium and each must have its start value set. When you manage to calculate equilibriums of such experimental points, this command is useful to transfer the site fractions from a successfully-calculated equilibria to the present experimental point.

| | |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | TRANSFER_START_VALUES |
| Prompt | <p>From equilibrium /Previous/: <Equilibrium number></p> <p>The equilibrium number is the numeric identifier for the equilibrium from which the start values should be copied to the present experimental point. <i>Previous</i> is the default if you press <Enter>.</p> |

Tabulation Reaction (TAB) Commands

In this section:

| | |
|----------------------------|-----|
| ENTER_FUNCTION | 322 |
| ENTER_REACTION | 323 |
| LIST_SUBSTANCES | 324 |
| SET_ENERGY_UNIT | 327 |
| SET_PLOT_FORMAT | 327 |
| SWITCH_DATABASE | 327 |
| TABULATE | 329 |
| TABULATE_DERIVATIVES | 329 |
| TABULATE_REACTION | 333 |
| TABULATE_SUBSTANCE | 336 |

ENTER_FUNCTION



This command is available with the GES and TAB modules.

Used to define a new thermodynamic function to be included in the sixth column of tabular output. The last entered function is listed in the 6th column of all tables, and can be plotted (if choosing the Plot Column value 6) in all graphs, for all subsequently tabulated substances or reactions.

| Syntax | ENTER_FUNCTION |
|---------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | Name: <Name> Function: <Definition> |
| | A limited number of state variables, G, H, S, T, P, V and H298 can be used in the function definition. For example, $-(G-H)/T$ can be defined as a function which is identical to S for a substance or ΔS for a reaction, $G+T*S-P*V$ can be defined as a function which is U (internal energy) for a substance or ΔU (internal energy change) for a reaction. |
| Options | Name of the function (maximum 8 characters) and Definition of the function. A long function can be typed over several lines. A function should be terminated by a semicolon (;) or an empty line. |

EXAMPLE OUTPUT

For the pure substance Fe (using the SSUB database), by entering a function as $G+T*S-P*V$, the following table is obtained by typing <Enter> in the prompt `Output file /Screen/:`, and the figure by typing 6 in the prompt `Plot column /2/:`

```
TAB: ENTER-FUNCTION
Name: InEnergy
Function: G+T*S-P*V;
TAB: TABULATE_SUBSTANCE
Substance (phase): Fe
Pressure /100000/: <Enter>
Low temperature limit /298.15/: <Enter>
High temperature limit /2000/: <Enter>
Step in temperature /100/: <Enter>
Output file /try1/: try2
Graphical output? /Y/: <Enter>
Plot column? /2/: 6
```

This gives the following output:

O U T P U T F R O M T H E R M O - C A L C

Column 6: InEnergy G+T*S-P*V

Phase : FE_S Pressure : 100000.00

Specie: FE

| T | Cp | H | S | G | InEnergy |
|-----------------------|-------------|-------------|-------------|--------------|----------------|
| (K) | (Joule/K) | (Joule) | (Joule/K) | (Joule) | |
| ***** | | | | | |
| 298.15 | 2.48446E+01 | 2.17972E-06 | 2.72800E+01 | -8.13353E+03 | 2.17972E-06 |
| 300.00 | 2.48905E+01 | 4.60049E+01 | 2.74338E+01 | -8.18414E+03 | 4.60049E+01 |
| 400.00 | 2.71299E+01 | 2.64957E+03 | 3.49085E+01 | -1.13138E+04 | 2.64957E+03 |
| 500.00 | 2.93561E+01 | 5.47211E+03 | 4.11976E+01 | -1.51267E+04 | 5.47211E+03 |
| 600.00 | 3.19293E+01 | 8.53245E+03 | 4.67701E+01 | -1.95296E+04 | 8.53245E+03 |
| 700.00 | 3.50985E+01 | 1.18777E+04 | 5.19207E+01 | -2.44667E+04 | 1.18777E+04 |
| 800.00 | 3.92042E+01 | 1.55830E+04 | 5.68623E+01 | -2.99068E+04 | 1.55830E+04 |
| 900.00 | 4.49645E+01 | 1.97726E+04 | 6.17903E+01 | -3.58387E+04 | 1.97726E+04 |
| 1000.00 | 5.42147E+01 | 2.46891E+04 | 6.69619E+01 | -4.22728E+04 | 2.46891E+04 |
| 1100.00 | 4.55851E+01 | 2.99025E+04 | 7.19412E+01 | -4.92328E+04 | 2.99025E+04 \$ |
| Stable phase is FE_S2 | | | | | |
| 1200.00 | 3.40840E+01 | 3.51037E+04 | 7.64466E+01 | -5.66322E+04 | 3.51037E+04 |
| 1300.00 | 3.49398E+01 | 3.85549E+04 | 7.92086E+01 | -6.44162E+04 | 3.85549E+04 |
| 1400.00 | 3.57994E+01 | 4.20918E+04 | 8.18293E+01 | -7.24692E+04 | 4.20918E+04 |
| 1500.00 | 3.66636E+01 | 4.57149E+04 | 8.43287E+01 | -8.07780E+04 | 4.57149E+04 |
| 1600.00 | 3.75330E+01 | 4.94247E+04 | 8.67226E+01 | -8.93314E+04 | 4.94247E+04 \$ |
| Stable phase is FE_S3 | | | | | |
| 1700.00 | 4.05217E+01 | 5.41173E+04 | 8.95609E+01 | -9.81363E+04 | 5.41173E+04 |
| 1800.00 | 4.12595E+01 | 5.82055E+04 | 9.18975E+01 | -1.07210E+05 | 5.82055E+04 \$ |
| Stable phase is FE_L | | | | | |
| 1900.00 | 4.60000E+01 | 7.74165E+04 | 1.02377E+02 | -1.17099E+05 | 7.74165E+04 |
| 2000.00 | 4.60000E+01 | 8.20165E+04 | 1.04736E+02 | -1.27456E+05 | 8.20165E+04 |

ENTER_REACTION



This command is for the TABULATE_REACTION (TAB) module.

This is the same as TABULATE_REACTION in that both the chemical reaction can be specified and the thermodynamic property changes for the reaction can be generated as a table, and plotted as a graph or saved as an experimental file (with an extension of .EXP). The thermodynamic data are automatically retrieved from the SSUB database (by default), or the current database set by SWITCH_DATABASE (thus there is no need to use the TDB module

before this command). You can select any other database by using the SWITCH_DATABASE command in the TAB module. The rules to specify a reaction are the same as TABULATE_REACTION.

| Syntax | ENTER_REACTION |
|---------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Same reaction? /Y/:</p> <p>This displays if there is at least one reaction already defined either by ENTER_REACTION or TABULATE_REACTION. For Y the next prompt for defining reaction is not asked.</p> |
| | <p>Reaction: <Chemical reaction equation> & <RA+RB=PC+PD></p> <p>A long reaction can be typed over several lines. A reaction should be terminated by a semicolon (;) or an empty line. A list showing the used database, defined elements, getting-data sequence, references, etc.:</p> <pre> Pressure /100000/: <Pressure of interest, in pa> Low temperature limit /298.15/: <T-low, in K> High temperature limit /2000/: <T-high, in K> Step in temperature /100/: <T-step> </pre> |
| | <p>Output file /Screen: <Return for screen, or type a file name></p> <p>If you type Return for screen a list of thermodynamic property changes for the defined/chosen reaction is shown up as a table (which is demonstrated in the example outputs given below), and the command is terminated.</p> <p>If typing a file name, the table is displayed and saved as an *.EXP or an *.TAB file. Then prompts:</p> |
| | <p>Graphical output /Y/:</p> <p>For N a table is output to the screen and this table is saved as a basic text file with the default extension .TAB under the current working directory. In this case, the graph cannot be plotted.</p> <p>By default a table is created with all thermodynamic functions as normal (which is displayed on screen) and generates a graph with temperature on the X-axis and a chosen property on a certain column in the table on the Y-axis (which is plotted on screen and saved as an *.EXP file). You are also prompted for the plot column.</p> |
| | <p>Plot column? /2/: <1 or 2 or 3 or 4 or 5 or 6></p> <p>Specify which property (as column number) to be plotted as the Y-axis (versus temperature as X-axis) as a graph on the screen. Simultaneously, all tabulated properties and the Y-axis setting (i.e. the plotted column) for the graph is written into an *.EXP file using the DATAPLOT format. The default column 2 is heat capacity, 3 enthalpy, 4 entropy and 5 Gibbs energy, and the additional column 6 is a user-entered function. The table displays on the screen. The plot then displays on the screen, followed by a POST prompt. The POST module (postprocessor) automatically opens, and all types of the POST-module commands to refine the plotted diagram may be used. Possibilities include scaling the X/Y-axis, changing the X/Y-axis texts, etc. The command BACK or EXIT at the POST prompt always takes you back to the TAB module.</p> |

LIST_SUBSTANCES



This command is for the TABULATE_REACTION (TAB) module.

List all species in the current database with a certain set of elements. This is useful to specify species as pure substances in the command ["TABULATE SUBSTANCE" on page 336](#).

| Syntax | LIST_SUBSTANCES |
|---------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>With elements <code>/*/ <*</code> or a set of elements></p> <p>The elements building up various species must be specified. The wildcard <code>*</code> means all elements in the current database.</p> <p>If some elements are specified, it also prompts for how to list species with such elements.</p> |
| | <p>Exclusively with those elements <code>/Y/</code>:</p> <p>All species (not phases) in the current database are searched. Keep the default (Y) if you do not want other elements included in the search except for those specified. Enter N to list all species containing at least one of the specified elements.</p> |

EXAMPLE OUTPUT

For the SSOL database, there are different lists, as shown below:

```
TAB: l-sub
With elements /*/: <Enter>
VA                AG                AL
AM                AS                AU
B                 BA                BE BI  BR C
CA                CD                CE
CL                CO                CR
CS                CU                DY
ER                EU                F
FE                GA                GD
GE                H                 HF
HG                HO                I
IN                IR                K
LA                LI                LU
MG                MN                MO
NA                NB
ND                NI                NP
OS                P
PA                PB                PD
PR                PT                PU
```

| | | |
|-------|---------|------------------|
| RB | RE | RH |
| RU | S | SB |
| SC | SE | SI |
| SM | SN | SR |
| TA | TB | TC |
| TE | TH | TI |
| TL | TM | U |
| V | W | Y |
| YB | ZN | ZR |
| C1 | C2 | C3 |
| C4 | C5 | C6 |
| C7 | N2 | O2 |
| P1 | P2 | P4 |
| NA/+1 | K/+1 | CL/-1 |
| H2O | H1/+ | LI1/+ |
| CS1/+ | RB1/+ | O1H1/- |
| F1/- | BR1/- | I1/- |
| H1/+1 | H1O1/-1 | SI1O2 CA1O1 TAB: |

TAB: l-sub

With elements /*/: fe cr ni c n o

Exclusively with those elements? /Y/: <Enter>

| | | |
|---|----|----|
| C | CR | FE |
| N | NI | O |
| C | C2 | C3 |
| C | C5 | C6 |
| C | N2 | O2 |

TAB:l-sub fe cr ni c n o

Exclusively with those elements? /Y/: n

| | | | |
|-----|--------|--------------------------|------|
| C | CR | FE N | NI O |
| C1 | C2 | C3 | |
| C4 | C5 | C6 | |
| C7 | N2 | O2 | |
| H2O | O1H1/- | H1O1/-1 SI1O2 CA1O1 TAB: | |

SET_ENERGY_UNIT

Set the energy unit as calories or Joule, in all the subsequent outputs (tables, graphs, and files) in the current calculation operation.

| | |
|--------|------------------------------------------|
| Syntax | SET_ENERGY_UNIT |
| Prompt | Energy unit (C=Cal, J=Joule) /J/: <Unit> |

SET_PLOT_FORMAT



This command is for the TABULATE_REACTION (TAB) module.

Set the plotting format while the result is plotted on screen or the file is saved as EXP file [using DATAPLOT graphical format] and TAB file (as a basic text file and as displayed on screen).



This command is different from SET_PLOT_FORMAT in the POST module, but is identical to SET_PLOT_ENVIRONMENT in the SYS (system utility) monitor.

| | |
|---------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | SET_PLOT_FORMAT |
| Options | The default set <code>Unit</code> is 1 (Windows) or 9 (Linux) for graphical presentation on screen, or all other units for outputs as *.EXP and *.TAB files. Also set the format of the graphical output to different graphical devices. The default unit 22 (1 for legacy Windows, and 9 for legacy Linux) may be altered with SET_PLOT_ENVIRONMENT in the SYS monitor or by the TC.INI file. |

SWITCH_DATABASE



This command is for the TABULATE_REACTION (TAB) module.

By default, the TAB module always automatically retrieves thermodynamic data for substances or reactant/product substances in a defined reaction, or for pure phases or ideal solution phases, from the SSUB Substances database. However, you can select thermodynamic data for complex non-ideal solution phases from another database, which is possible with this command.

| | |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | SWITCH_DATABASE |
| Prompt | Database /XYZ/: <new database name> Specify a New database name. XYZ stands for the default SSUB database or the current database which is switched on. |

| Syntax | SWITCH_DATABASE |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>If an appropriate database name is not given and the <code>USER</code> option is not used, a list displays of available databases.</p> <p>Use one of these databases:</p> <ul style="list-style-type: none"> • PURE = SGTE Pure Elements Database • SSUB = SGTE Substances Database • USER = user defined database |

This command switches (or changes) from the current database to a new one, and reinitializes the entire TAB module for defining a substance or reaction and the GIBBS workspace for storing retrieved data. All the directly connected databases as predefined by the original database initiation file `tc_initd.tdb` are listed by pressing the <Enter> key without giving any argument. You can also supply your own database by giving the argument `USER` and then the database name and, if it is not located in the current working directory, its correct path.

This command (when required to use another database for subsequent tabulations) must be used before executing the TAB commands `TABULATE_SUBSTANCE` for substances, and `ENTER_REACTION` or `TABULATE_REACTION` for reactions.

When a predefined database or an appropriate `USER` database is switched on, the `DATA` command `GET_DATA` is automatically executed.

DATABASE NAME: The new database is specified by typing the abbreviation given in the front of one of the available predefined databases. For convenience when switching/appending databases you can add them to the predefined database list in the database initiation file `tc_initd.tdb` of your installed software.

When this command is used in a macro (*.TCM) file, if the `USER` option is selected, the database setup file name (*setup.TDB) containing the setup definitions of the user database, and its correct path, must be provided.

If a `USER` database name or its path is not given on the same line of the `SWITCH_DATABASE` command, or if it is incomplete or incorrect, an Open window displays to specify the filename of the database setup file name (*setup.TDB) of the to-be-switched `USER` database.



Unlike in the TDB module, if a user database is chosen, the Gibbs energy system is also reinitialized and only data from the user databases are retrieved for tabulations.

After this command, those commands to define systems (in terms of either elements or species), to reject/restore phases or species, retrieve data, as well as to append data from additional database(s), can be done.

TABULATE



This command is for the TABULATE_REACTION (TAB) module.

Gives the values of an already-defined table (with various properties varied with the stepping axis variable) from equilibria calculated with a STEP command. You can tabulate a table even if the table is entered after the step calculation.

| Syntax | TABULATE |
|---------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | Name: <Name of a defined table> The name of the table must be given. The table must be entered. |
| | Output to Screen or file /Screen/: <File name> The table can be listed on the screen (by pressing <Enter>), on a file (the file name must be specified here). |

TABULATE_DERIVATIVES



This command is for the TABULATE_REACTION (TAB) module.




This command is mainly for system debugging purposes and for experienced users. It automatically calculates all partial derivatives for a pure phase or solution phase at a given composition.



This is not the same as the chemical potential.

Before using this command, the system must be defined and thermodynamic data retrieved from an appropriate solution database in the TDB module. The phase name can be given in either upper, lower or mixed cases, and can be abbreviated until it is unique, e.g. fcc, BCC, cem, Liq, etc. as the SSOL database is used for the tabulations, or GAS, FE-S, wustite, Fe2O3-hem, etc. as the SSUB database is used. The module then optionally goes through a specific sublattice or all the possible sublattices for the specified phase, as well as through the whole framework of a currently defined system (including all the defined elements/species, as well as the default defined vacancy and electron if necessary for the current database), when it prompts for inputs of site fractions for various species possibly occupying such sublattices.

Therefore, thermodynamic properties can be tabulated for a pure phase, or for a solution phase as a pure end-member (with a composition definition for the corresponding non-interacting species on all necessary sublattices in the end-member), or for a solution phase as a real solution (with a composition definition for related interacting species on all necessary sublattices in the solution).

| Syntax | TABULATE_DERIVATIVES |
|---------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Phase name /XXXX/: <Name of the phase></p> <p>Specify the phase name of a pure phase or a solution phase.</p> <p>XXXX is the last phase the TAB module accounted for. It automatically prompts for other options and necessary inputs for the definition of the composition of the specified phase.</p> <p>For a pure phase (such as Fe-S, Wustite, and Fe2O3-Hematite), no further composition definition is needed. For a solution phase with one sublattice (such as AQUEOUS solution, GAS mixture and SLAG solution), it requests $n-1$ site-fraction inputs for the phase constituents (if there are n species in the defined phase within the whole framework of currently defined system, including all the defined elements/species, as well as the default defined vacancy and electron if necessary for the current database); the nth species is automatically assigned as the rest.</p> <div>  <p>The sum of input site fractions must not exceed unity.</p> </div> |
| | <p>EXAMPLE</p> <p>For example, these prompts and inputs can be seen for a LIQUID solution phase (from the SSOL database) within the Fe-Cr-Ni-C-N-O framework (Note that by default, the unprompted Ni species are assigned as the rest):</p> <pre> FRACTION OF CONSTITUENT (RETURN FOR PROMPT): <RETURN> C /1/: .05 CR /1/: .1 FE /1/: < RETURN> SUM OF FRACTIONS EXCEED UNITY, PLEASE REENTER FE /1/: .8 N /1/: .005 </pre> <p>For a solution phase with two or more sublattices (such as FCC alloy solution, and ION_LIQ ionic liquid solution), it first asks for which sublattice the site-fractions of constituents shall be specified: the default value 0 for all possible sublattices, and a given positive number for a specific sublattice (of course, this number must be reasonable for the currently specified phase, i.e. it must be smaller than the total sublattice number of the phase). Then, for the given sublattice or for all sublattices, it prompts for all the necessary inputs of site-fractions for the possible constituents on each sublattice $n-1$ times if there are n species on such a sublattice in the defined phase; the nth species on each of the sublattices is automatically assigned as the rest. For example, the following prompts and inputs can be seen for an FCC solution phase (from the SSOL database) within the Fe-Cr-Ni-C-N-O framework (Note that by default, the unprompted O species on its sublattice 1 and VA on its sublattice 2 are assigned as the rest):</p> <pre> SPECIFY SUBLATTICE (0 FOR ALL) /0/: <RETURN> </pre> |

| Syntax | TABULATE_DERIVATIVES |
|--------|----------------------------------------------------------------------------------------------------------------------------|
| | <pre> FRACTIONS IN SUBLATTICE 1 CR /1/: .1 FE /1/: .8 NI /1/: .0995 FRACTIONS IN SUBLATTICE 2 C /1/: .05 N /1/: .05 </pre> |
| | <p>Temperature /2000/: <Temperature of interest, in K></p> <p>Specify the temperature of interest in K.</p> |
| | <p>Pressure /100000/: <Pressure of interest, in pa></p> <p>Specify the pressure of interest in Pa.</p> |

EXAMPLE OUTPUT

For the FCC phase in the Fe-Cr-Ni-C-N-O system (using the SSOL database), the following table is obtained at a specified composition:

```

TAB: TAB_DER
Phase name /BCC/: FCC
SPECIFY SUBLATTICE (0 FOR ALL) /0/: <Enter>
FRACTIONS IN SUBLATTICE 1
CR /1/: .1
FE /1/: .8
NI /1/: .3
SUM OF FRACTIONS EXCEED UNITY, PLEASE REENTER
NI /0/: .0995
FRACTIONS IN SUBLATTICE 2
C /1/: .05
N /1/: .05
Temperature /1800/: <Enter>
Pressure /100000/: <Enter>
Gibbs energy: ..... -1.27432533E+05
Helmholz energy: ..... -1.27433205E+05
Enthalpy: ..... 5.95773994E+04
Internal energy: ..... 5.95767279E+04
Entropy: ..... 1.03894407E+02

```

```

Molar volume: ..... 6.71473258E-06
Thermal expansivity: ..... 7.63886416E-05
Isothermal compressibility: ..... 6.02925387E-12
Heat capacity at constant pressure: 4.33555074E+01
First partial derivative with respect to CR in sublattice 1 of Gibbs energy:
..... -1.26034739E+05 of enthalpy: .....
4.63000206E+04 of entropy: ..... 9.57415334E+01 of volume:
..... 6.87203263E-06
Second partial derivative of Gibbs energy with respect to also
CR in 1: 1.54392858E+05
FE in 1: -1.53353158E+04
NI in 1: -1.71750366E+04
O in 1: 0.00000000E+00
C in 2: -1.82016870E+05
in 2: -3.73062665E+05
VA in 2: -9.36260878E+04
first partial derivative with respect to FE in sublattice 1 of Gibbs energy:
..... -1.02869265E+05
of enthalpy: ..... 6.11738912E+04 of entropy:
..... 9.11350866E+01 of volume: .....
7.53441165E-06
Second partial derivative of Gibbs energy with respect to also
FE in 1: 1.82508696E+04
NI in 1: -3.07043434E+03
in 1: 0.00000000E+00
C in 2: -1.36027071E+05
in 2: -2.13007485E+05
VA in 2: -1.11741180E+05
First partial derivative with respect to NI in sublattice 1 of Gibbs energy:
..... -1.32427029E+05 of enthalpy: .....
5.21563580E+04 of entropy: ..... 1.02546326E+02 of volume:
..... 0.00000000E+00
Second partial derivative of Gibbs energy with respect to also
NI in 1: 1.48390257E+05
in 1: 0.00000000E+00
C in 2: -7.70620431E+04
in 2: -1.61551726E+05
VA in 2: -1.12772206E+05

```

```

First partial derivative with respect to O in sublattice 1      of Gibbs energy:
..... -2.62929308E+05      of enthalpy: .....
5.02555370E+04      of entropy: ..... 1.73991581E+02      of volume:
..... 0.00000000E+00

Second partial derivative of Gibbs energy with respect to also
in 1: 2.99322360E+07

C                      in 2: 0.00000000E+00
N                      in 2: 0.00000000E+00
VA                     in 2: -1.82377137E+05

First partial derivative with respect to C in sublattice 2      of Gibbs energy:
..... -1.59508417E+05      of enthalpy: .....
1.21269096E+05      of entropy: ..... 1.55987507E+02      of volume:
..... 1.06885187E-05

Second partial derivative of Gibbs energy with respect to also
C                      in 2: 2.99322360E+05
N                      in 2: -1.90144000E+04
VA                     in 2: -2.78465070E+04

First partial derivative with respect to N in sublattice 2      of Gibbs energy:
..... -2.39671400E+05      of enthalpy: .....
4.04456947E+04      of entropy: ..... 1.55620608E+02      of volume:
..... 0.00000000E+00

Second partial derivative of Gibbs energy with respect to also
N                      in 2: 2.99322360E+05
VA                     in 2: -3.30383665E+04

First partial derivative with respect to VA in sublattice 2      of Gibbs energy:
..... -9.52042686E+04      of enthalpy: .....
5.37142294E+04      of entropy: ..... 8.27324989E+01      of volume:
..... 6.86700739E-06

Second partial derivative of Gibbs energy with respect to also
VA                     in 2: 1.66290200E+04

```

TABULATE_REACTION



This command is for the TABULATE_REACTION (TAB) module.

Tabulate thermodynamic property changes for a chemical reaction as a table, or variation of one chosen property can be plotted against temperature as a graph, or saved as an experimental file (with an extension of .EXP). The thermodynamic data are automatically retrieved from the SSUB5 database (by default), or the current database set by the SWITCH_DATABASE command (thus there is no need to use the DATA module before this command). You can select any other database by using SWITCH_DATABASE.

It is important to remember the rules to specify a reaction:

- The reaction is specified, by giving the reactants and products, such as $\text{Ga}+\text{S}=\text{GaS}$, $5\text{Al}+2\text{Fe}=\text{Al}_5\text{Fe}_2$.
- Under Linux environments, the notation for a chemical formula treats upper and lower cases as the same (such as $\text{ga}+\text{s}=\text{GaS}$, $5\text{Al}+2\text{Fe}=\text{al}_5\text{fe}_2$); but under Windows, the TAB module only accepts upper cases, e.g. $\text{GA}+\text{S}=\text{GAS}$, $5\text{AL}+2\text{FE}=\text{AL}_5\text{FE}_2$.
- Elements with a single letter symbol must be followed by a stoichiometry factor, even if it is 1; thus, the symbol Co is taken as cobalt, carbon monoxide must be given as C1O1 (or O1C1).
- All the reactants and products must be defined as species-stoichiometries in the currently-used database; in other words, the reaction definition only accepts already-defined species-stoichiometries as reactants and products. For example, if a database does not have a species defined with a stoichiometry of Al_5Fe_2 {e.g. the Al and Fe (but not Al_5Fe_2) may be defined as species, and the Al_5Fe_2 phase may be defined as a two-sublattice stoichiometric phase $[\text{Al}]_5[\text{Fe}]_2$, rather than a single sublattice stoichiometric phase $[\text{Al}_5\text{Fe}_2]$ }, then the reaction $5\text{Al}+2\text{Fe}=\text{Al}_5\text{Fe}_2$ cannot be tabulated.
- Make sure that the Gibbs free energy expression for a stoichiometric phase is really corresponding to the species-stoichiometry. For example, if a database has a definition of Function GAL_5FE_2 for 1/7 of the Al_5Fe_2 formula, then the relation $\text{G}(\text{Al}_5\text{Fe}_2)=7*\text{GAL}_5\text{FE}_2$ must be defined; otherwise, the tabulated thermodynamic properties for the reaction $5\text{Al}+2\text{Fe}=\text{Al}_5\text{Fe}_2$ is wrong.

| Syntax | TABULATE_REACTION |
|---------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Same reaction? /Y/:</p> <p>This prompt displays if there is at least one reaction already defined either with the commands ENTER_REACTION or TABULATE_REACTION. The following prompts only display if N is entered.</p> <p>Reaction: <Chemical reaction equation> & <RA+RB=PC+PD></p> <p>A long reaction can be typed over several lines. A reaction should be terminated by a semicolon (;) or an empty line. A list showing the used database, defined elements, getting-data sequence, references, etc.</p> <p>Pressure /100000/: <pressure of interest, in pa></p> <p>Low temperature limit /298.15/: <T-low, in K> Specify the starting temperature K.</p> <p>High temperature limit /298.15/: <T-high, in K> Specify the ending temperature K.</p> <p>Step in temperature /100/: <T-step> Specify the temperature step for the tabulation.</p> <p>Output file /Screen/: <Return for screen, or type a file name></p> <p>If you type Return for screen, a list of thermodynamic property changes for the defined/chosen reaction is shown as a table (which is demonstrated in the example outputs given below), and the command is terminated.</p> <p>If typing a file name, the table is both displayed on screen and saved as an *.EXP or a *.TAB file, and the program prompts:</p> |

| Syntax | TABULATE_REACTION |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>Graphical output /Y/:</p> <ul style="list-style-type: none"> For N a table is output to the screen, and the same table is saved as a basic text file with the default extension .TAB under the current working directory. In this case, the graph cannot be plotted. For Y a table is created with all thermodynamic functions as normal (which is displayed on screen) and generates a graph with temperature on the X-axis and a chosen property on a certain column in the table on the Y-axis (which is plotted on screen and saved as an *.EXP file), and it also asks which column is to be plotted on the resulting graph: |
| | <p>Plot column? /2/: <1 or 2 or 3 or 4 or 5 or 6></p> <p>Specify which property (as column number) to be plotted as the Y-axis (versus temperature as X-axis) as a graph on the screen. Simultaneously, all tabulated properties and the Y-axis setting (i.e. the plotted column) for the graph is written into an *.EXP file using the DATAPLOT format. The default column 2 is heat capacity, 3 enthalpy, 4 entropy and 5 Gibbs energy, and the additional column 6 is a user-entered function. The table displays on the screen. The plot then displays on the screen, followed by a POST: prompt. The POST module automatically opens, and all types of the POST module commands to refine the plotted diagram may be used. Possibilities include scaling the X/Y-axis, changing the X/Y-axis texts, etc. The command BACK or EXIT at the POST: prompt always takes you back to the TAB module.</p> |

EXAMPLE OUTPUT

For the reaction $\text{Ga} + \text{S} = \text{GaS}$ (using the SSUB database), the following table is obtained by typing <Enter> in the prompt Output file /SCREEN/, and the figure by typing 2 in the prompt

Plot column /2/:

```

O U T P U T   F R O M   T H E R M O - C A L C
Reaction:  S+GA=GA1S1
stable as S_S
GA stable as GA_S
GA1S1 stable as GA1S1_S
Delta-Cp      Delta-H      Delta-S      Delta-G
(K)      (Joule/K)      (Joule)      (Joule/K)      (Joule)
*****
298.15  -2.79489E+00  -2.09200E+05  -1.50580E+01  -2.04710E+05
300.00  -2.87516E+00  -2.09205E+05  -1.50755E+01  -2.04683E+05
302.    ---- GA becomes GA_L ,delta-H =    5589.80
367.    ---- S becomes S_S2 ,delta-H =    401.00
389.    ---- S becomes S_L ,delta-H =    1721.00
400.00  -1.22278E+01  -2.17521E+05  -4.07488E+01  -2.01222E+05

```

| | | | | |
|---------|--------------|--------------|--------------|--------------|
| 500.00 | -1.57686E+01 | -2.19323E+05 | -4.47280E+01 | -1.96959E+05 |
| 600.00 | -1.02518E+01 | -2.20583E+05 | -4.70410E+01 | -1.92359E+05 |
| 700.00 | -6.58954E+00 | -2.21430E+05 | -4.83534E+01 | -1.87583E+05 |
| 800.00 | -4.46246E+00 | -2.21963E+05 | -4.90686E+01 | -1.82709E+05 |
| 900.00 | -2.82671E+00 | -2.22328E+05 | -4.94995E+01 | -1.77778E+05 |
| 1000.00 | -1.21787E+00 | -2.22530E+05 | -4.97138E+01 | -1.72816E+05 |
| 1100.00 | 3.71702E-01 | -2.22572E+05 | -4.97552E+01 | -1.67841E+05 |

TABULATE_SUBSTANCE



This command is for the TABULATE_REACTION (TAB) module.

Tabulate thermodynamic properties of a substance (with a given chemical formula but it is not certain in which phase/state it may form) or a pure stoichiometric phase (getting data from a specific substance database such as SSUB, or from a specific solution database such as SSOL and TCFE), or of a solution phase with a fixed composition (getting data from a specific solution database such as SSOL and TCFE), under a constant pressure and various temperatures.

In case of a pure stoichiometric phase or a solution phase with a fixed composition, you must already define the system and get thermodynamic data from an appropriate solution database in the TDB module before using this TAB command. The phase name can be given either upper or lower or mixed cases, and can be abbreviated until it is unique, e.g. *fcc*, *BCC*, *Liq*, *cem*, *Al5Fe2*, etc. as the SSOL database is used for the tabulations, or *GAS*, *FE-S*, *wustite*, *Fe2O3-hem*, etc. as the SSUB database is used. The module then optionally goes through a specific sublattice or all the possible sublattices for the specified phase, as well as through the whole framework of a currently defined system (including all the defined elements/species, as well as the default defined vacancy and electron if necessary for the current database), when it prompts for inputs of site fractions for various species possibly occupying such sublattices. Therefore, you can tabulate thermodynamic properties for a pure phase, or for a solution phase as a pure end-member (with a composition definition for the corresponding non-interacting species on all necessary sublattices in the end-member), or for a solution phase as a real solution (with a composition definition for related interacting species on all necessary sublattices in the solution).

Moreover, the variation for one of the tabulated properties for a substance, a pure stoichiometric phase, or a solution phase with a fixed composition can be plotted against temperature as a graph or saved as an experimental file (with an extension of .EXP).

| Syntax | TABULATE_SUBSTANCE |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | Substance (phase): <Name of the species or phase> In case of a substance, give its chemical formula, e.g. Fe, H2, C1H6, FeC1, CaC1O3, MgSiO3, etc. |

| Syntax | TABULATE_SUBSTANCE |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>When the TABULATE_SUBSTANCE <SUBSTANCE> command sequence is used for the first time in the TAB module, it always uses the SSUB Substances database as the default. If SSUB is not available and a specific database has not been switched on yet, it may prompt to specify an appropriate substance or solution database (e.g. typing SSUB<version number>; SSOL<version number>; TCFE<version number> etc.). Prior to this command, you can also use SWITCH_DATABASE to set the current database. If a solution database is set as the current database, only the neutral species that are valid substance standing by themselves as phases can be tabulated.</p> <div>  <p>Before other prompts, a list of the used database, defined elements, getting-data sequence, references, etc. is displayed on screen. From such information, you know what the TAB module is performing.</p> </div> <p>In case of a pure stoichiometric phase or a solution phase, give its phase name, e.g. FCC, CEMENTITE, LIQUID, SLAG, AQUEOUS, GAS, Al₅Fe₂, Fe-S, Wustite, Fe₂O₃-Hematite, etc.</p> <div>  <p>REMEMBER: It is important that you have already defined the system and gotten thermodynamic data from an appropriate solution database in the TDB module before using this TAB_SUB command. It automatically prompts for other options and necessary inputs for the definition of the composition of the specified phase.</p> </div> <p>For a pure stoichiometric phase defined with one single sublattice (such as Fe-S, Wustite, and Fe₂O₃-Hematite), no further composition definition is needed.</p> <p>For a solution phase defined with one sublattice (such as AQUEOUS solution, GAS mixture and SLAG solution), it requests n-1 site-fraction inputs for the phase constituents (if there are <i>n</i> species in the defined phase within the whole framework of currently defined system, including all the defined elements/species, as well as the default defined vacancy and electron if necessary for the current database); the <i>n</i>th species is automatically assigned as the rest.</p> <div>  <p>The sum of input site fractions must not exceed unity. For example, the following prompts and inputs can be seen for a LIQUID solution phase (from the SSOL database) within the Fe-Cr-Ni-C-N-O framework (Note that by default, the unprompted Ni species is assigned as the rest):</p> </div> <pre> Fraction of constituent (return for prompt): <Return> C /1/: .05 CR /1/: .1 FE /1/: <RETURN> Sum of fractions exceed unity, please reenter FE /1/: .8 N /1/: .005 </pre> |

| Syntax | TABULATE_SUBSTANCE |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>For a pure stoichiometric phase defined with two or more sublattices (such as Al₅Fe₂ inter-metallic stoichiometric phase) and for a solution phase defined with two or more sublattices (such as FCC alloy solution, and ION_LIQ ionic liquid solution, Al₅Fe₄ inter-metallic solution phase), it first asks for which sublattice the site-fractions of constituents shall be specified: the default value 0 for all possible sublattices, and a given positive number for a specific sublattice (this number must be reasonable for the currently specified phase, i.e. it must be smaller than the total sublattice number of the phase). Then, for the given sublattice or for all sublattices, it prompts for all the necessary inputs of site-fractions for the possible constituents on each sublattice $n-1$ times if there are n species on such a sublattice in the defined phase; the nth species on each of the sublattices are automatically assigned as the rest. For example, these prompts and inputs can be seen for an FCC solution phase (from the SSOL database) within the Fe-Cr-Ni-C-N-O framework (Note that by default, the unprompted \circ species on its sublattice 1 and v_A on its sublattice 2 is assigned as the rest):</p> |
| | <pre>Specify sublattice (0 for all) /0/: FRACTIONS IN SUBLATTICE 1 CR /1/: .1 FE /1/: .8 NI /1/: .0995 FRACTIONS IN SUBLATTICE 2 C /1/: .05 N /1/: .05</pre> |
| | <p>Pressure /100000/: <Pressure of interest, in pa></p> <p>Specify the constant pressure condition in Pa.</p> |
| | <p>Low temperature limit /298.15/: <T-low, in K></p> <p>Specify the starting temperature K.</p> |
| | <p>High temperature limit /298.15/: <T-high, in K></p> <p>Specify the ending temperature K.</p> |
| | <p>Step in temperature /100/: <T-step> Specify the temperature step for the tabulation.</p> |
| | <p>Output file /Screen/: <Return for screen, or type a file name></p> <p>If you type <code>Return for screen</code> a list of basic thermodynamic functions for the chosen substance or for the specified pure or solution phase with the fixed composition is shown up as a table (which is demonstrated in the example outputs given below), and the command is terminated.</p> <p>If typing a file name, the table is both displayed on screen and saved as an *.EXP or a *.TAB file, and the program further prompts:</p> |
| | <p>Graphical output /Y/:</p> <ul style="list-style-type: none"> • For N a table is output to the screen, and the same table is saved as a basic text file with the default extension .TAB under the current working directory. In this case, the graph cannot be plotted. • For Y a table is created with all the thermodynamic functions as normal (which is displayed on |

| Syntax | TABULATE_SUBSTANCE |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | screen) as well as generates a graph with temperature on the X-axis and a chosen property on a certain column in the table on the Y-axis (which is plotted on screen and saved as an *.EXP file), and it also ask which column is to be plotted on the resulting graph: |
| | <p>Plot column ? /2/: <1 or 2 or 3 or 4 or 5 or 6></p> <p>Specify which property (as column number) to be plotted as the Y-axis (versus temperature as X-axis) as a graph on the screen. Simultaneously, all tabulated properties and the Y-axis setting (i.e. the plotted column) for the graph is written into an *.EXP file using the DATAPLOT format. The default column 2 is heat capacity, 3 enthalpy, 4 entropy and 5 Gibbs energy, and the additional column 6 is a user-entered function. The table displays on the screen. The plot then displays on the screen, followed by a POST: prompt. The POST module (postprocessor) automatically opens, and all types of the POST-module commands to refine the plotted diagram may be used. Possibilities include scaling the X/Y-axis, changing the X/Y-axis texts, etc. The command BACK or EXIT at the POST: prompt always takes you back to the TAB module.</p> |

EXAMPLE OUTPUT 1

For the FCC alloy phase as a non-ideal solution with a fixed composition

[Fe0.80,Cr0.10,Ni0.0995,O0.005][C0.05,N0.05,VA0.90]

The following table is obtained by typing Return for screen at the prompt Output file /SCREEN/:

```

O U T P U T   F R O M   T H E R M O - C A L C
Phase : FCC                                Pressure :      100000.00
Specie: CR1/--2
*****
      T           Cp           H           S           G
      (K)        (Joule/K)    (Joule)    (Joule/K)    (Joule)
*****
298.15   2.70517E+01   6.23824E+03   4.40241E+01  -6.88755E+03
300.00   2.70889E+01   6.28832E+03   4.41916E+01  -6.96915E+03
400.00   2.87304E+01   9.08420E+03   5.22235E+01  -1.18052E+04
500.00   2.99904E+01   1.20222E+04   5.87742E+01  -1.73649E+04
600.00   3.10889E+01   1.50770E+04   6.43408E+01  -2.35275E+04
700.00   3.21116E+01   1.82375E+04   6.92106E+01  -3.02100E+04
800.00   3.30994E+01   2.14982E+04   7.35633E+01  -3.73524E+04
900.00   3.40742E+01   2.48569E+04   7.75182E+01  -4.49094E+04
1000.00  3.50483E+01   2.83130E+04   8.11586E+01  -5.28456E+04

```

| | | | | |
|---------|-------------|-------------|-------------|--------------|
| 1100.00 | 3.60268E+01 | 3.18667E+04 | 8.45449E+01 | -6.11327E+04 |
| 1200.00 | 3.70143E+01 | 3.55187E+04 | 8.77219E+01 | -6.97476E+04 |
| 1300.00 | 3.80149E+01 | 3.92700E+04 | 9.07241E+01 | -7.86713E+04 |
| 1400.00 | 3.90311E+01 | 4.31222E+04 | 9.35784E+01 | -8.78875E+04 |
| 1500.00 | 4.00649E+01 | 4.70768E+04 | 9.63064E+01 | -9.73827E+04 |
| 1600.00 | 4.11174E+01 | 5.11358E+04 | 9.89256E+01 | -1.07145E+05 |
| 1700.00 | 4.21896E+01 | 5.53010E+04 | 1.01450E+02 | -1.17165E+05 |
| 1800.00 | 4.33555E+01 | 5.95774E+04 | 1.03894E+02 | -1.27433E+05 |
| 1900.00 | 4.58528E+01 | 6.40379E+04 | 1.06306E+02 | -1.37943E+05 |
| 2000.00 | 4.75402E+01 | 6.87138E+04 | 1.08704E+02 | -1.48694E+05 |

EXAMPLE OUTPUT 2



For a phase, as either an end-member or real solution, the listed species name is irrelevant.

For the H2 species as a pure substance (using the SSUB5 database), the following table is obtained by typing `Return for screen` at the prompt `Output file /SCREEN/`, whilst the figure is generated by typing `5` at the prompt `Plot column /2/`:

```

O U T P U T F R O M T H E R M O - C A L C
Phase : GAS                      Pressure :      100000.00
Specie: H2
*****
H          S          G          T          Cp
(K)      (Joule/K)    (Joule)    (Joule/K)    (Joule)
*****
2.88369E+01  3.17684E-06  1.30680E+02  -3.89622E+04  298.15
300.00    2.88473E+01  5.33580E+01  1.30858E+02  -3.92042E+04
400.00    2.91591E+01  2.95686E+03  1.39209E+02  -5.27268E+04
500.00    2.92650E+01  5.87874E+03  1.45729E+02  -6.69856E+04
600.00    2.93441E+01  8.80908E+03  1.51071E+02  -8.18336E+04
700.00    2.94579E+01  1.17488E+04  1.55602E+02  -9.71730E+04
800.00    2.96320E+01  1.47027E+04  1.59547E+02  -1.12935E+05
900.00    2.98786E+01  1.76776E+04  1.63050E+02  -1.29068E+05
1000.00   3.02043E+01  2.06810E+04  1.66214E+02  -1.45533E+05
1100.00   3.05319E+01  2.37171E+04  1.69108E+02  -1.62302E+05

```

| | | | | |
|---------|-------------|-------------|-------------|--------------|
| 1200.00 | 3.09281E+01 | 2.67897E+04 | 1.71781E+02 | -1.79348E+05 |
| 1300.00 | 3.13615E+01 | 2.99040E+04 | 1.74274E+02 | -1.96652E+05 |
| 1400.00 | 3.18115E+01 | 3.30625E+04 | 1.76614E+02 | -2.14197E+05 |
| 1500.00 | 3.22641E+01 | 3.62664E+04 | 1.78824E+02 | -2.31970E+05 |
| 1600.00 | 3.27094E+01 | 3.95151E+04 | 1.80921E+02 | -2.49958E+05 |
| 1700.00 | 3.31406E+01 | 4.28078E+04 | 1.82917E+02 | -2.68151E+05 |
| 1800.00 | 3.35526E+01 | 4.61426E+04 | 1.84823E+02 | -2.86539E+05 |
| 1900.00 | 3.39415E+01 | 4.95175E+04 | 1.86648E+02 | -3.05113E+05 |
| 2000.00 | 3.43045E+01 | 5.29300E+04 | 1.88398E+02 | -3.23866E+05 |

REACTOR (REACTOR_SIMULATOR) Commands

In this section:

| | |
|-----------------------------|-----|
| CREATE_DIVIDERS | 343 |
| CREATE_PIPES | 343 |
| CREATE_STAGE_BOXES | 344 |
| EXECUTE_POLY3_COMMAND | 345 |
| LIST_RECORDS | 345 |
| READ_WORKSPACE | 346 |
| SAVE_WORKSPACES | 346 |
| START_SIMULATION | 347 |

CREATE_DIVIDERS



This command is for the REACTOR_SIMULATOR (REACTOR) module.

Define the segment boundaries and the ways on how to distribute phases between various segments and to split the feeds of heat and mass.

| Syntax | CREATE_DIVIDERS |
|---------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | Number of dividers /4/: <The number of dividers> |
| | Specify the number of dividers (boundaries between various segments) in the reactor. It is normally the segment number plus one: for example, if the stage box number is defined as 4, the divider number should be defined as 5. |
| | Number of outputs for divider # /3/: <The number of outputs> |
| | Specify the number of outputs for a specific divider #. |
| | Percent of input to output 1 /100/: <Percent of input> |
| | Define the percentage of input to the output 1 in the current divider #. |
| | Percent of input to output ## /100/: <Percent(s) of input(s)> |
| | Define the percentages of inputs to the outputs ## in the current divider #. It is repeated till the last output is specified. |

CREATE_PIPES



This command is for the REACTOR_SIMULATOR (REACTOR) module.

Define the pipes between various segments and the ways on how the mass and heat transport between the surroundings (with the record number as 0) and the reactor, among various segments in the reactor, and along various dividers (segment boundaries in the reactor).

| Syntax | CREATE_PIPES |
|---------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | From record: <A record number> |
| | Specify a record number. If there are four segments in the reactor, these records are available: <ul style="list-style-type: none">• 0 surroundings• 1-4 stage boxes (segments)• 5-9 dividers (segment boundaries) |
| | Pipe to record: <Another record number> |
| | Specify another record number to which the mass or heat flows from the current record (specified above). Before this prompt, a message shown on the screen indicates what kind of |

| | |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | CREATE_PIPES |
| | mass or heat flow (according to the definitions of stage boxes and dividers, which have already been created prior to this command) should be specified in the pipe. This is repeated for all inputs and/or outputs for mass and/or heat in current record. |

CREATE_STAGE_BOXES



This command is for the REACTOR_SIMULATOR (REACTOR) module.

Create several reaction stages as boxes (segments), where the you define the feed in either mass input and initial temperature or heat input from surroundings, as well as the mass out and initial temperature in each of the segments.

| | |
|---------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | CREATE_STAGE_BOXES |
| Prompts | <p>Number of stage boxes /4/: <The number of stage boxes></p> <p>Specify the number of stage boxes in the reactor. Then define the feed of mass and/or energy (from surroundings to) the rector.</p> <p>Give feed to system: <Feed></p> <p>One feed (of mass or heat) to the reactor must be specified here. Two types of feeds can be used:</p> <ul style="list-style-type: none"> • As input amount of heat (enthalpy): H=Value. • As input amount of specific species or element and its initial temperature: N (SPECIES)=Value, Input temperature (in one line, or the input temperature in the next prompt). <p>Input temperature /298.15/: <Input temperature></p> <p>Give feed to system: <Feed></p> <p>Specify other feeds (mass or energy) to the reactor. Press <Enter> to finish the feed inputs, and then:</p> <p>Give for stage box #</p> <p>Now start to define the type of stage box (segment is specifically numbered as #), and to specify a guess of initial temperature and an output for each phase in the segment.</p> <p>Type of box/Equilibrium/: <Type of box></p> <p>Only the EQUILIBRIUM type is allowed. Press <Enter> to accept it.</p> <p>Is the stage heat controlled? /Y/: <Yes or No></p> <p>Y means the current segment is heat controlled.</p> <p>Initial guess of temperature? /1000/: <Initial temperature></p> <p>Give a guess of initial temperature (in K) for the current segment; press <Enter> to accept the default.</p> |

| Syntax | CREATE_STAGE_BOXES |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>Give initial amount: <Initial amount of mass or heat></p> <p>The initial amount of mass and/or heat in the current segment can be specified here. Two types of initial amount can be used:</p> <ul style="list-style-type: none"> • As initial amount of heat (enthalpy): H=Value. • As initial amount of specific species or element and its initial temperature: N (SPECIES)=Value, Input temperature (in one line, or the input temperature in the next prompt). |
| | Input temperature /298.15/: <Input temperature> |
| | <p>Give initial amount: <Initial amount of mass or heat></p> <p>Specify initial amount (mass or energy) in the current segment. Press <Enter> to finish the initial amount inputs, and then this message displays:</p> <p>Each phase may have a separate output, give these</p> <p>Now start to define the output for each phase.</p> |
| | <p>Phase name /Rest/: <Name of phase></p> <p>Specify a phase that has a separate output, e.g. GAS; by pressing <Enter> to accept that all REST phases do not have separate outputs. Then the program asks for further definitions of all the other segments (one by one), repeating some of the above questions, till the last segment in the reactor is defined.</p> |

EXECUTE_POLY3_COMMAND



This command is for the REACTOR_SIMULATOR (REACTOR) module.

| Syntax | EXECUTE_POLY3_COMMAND |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>To directly use all kinds of POLY commands inside the REACTOR module. Any legal POLY commands can be entered.</p> <p>▶ "POLY Module Commands" on page 131</p> |

LIST_RECORDS



This command is for the REACTOR_SIMULATOR (REACTOR) module.

| Syntax | LIST_RECORDS |
|--------|-------------------------------------------------------------------------------------------------------|
| | Lists all the already-created records for the reactor (including stage boxes, dividers, pipes, etc.). |

READ_WORKSPACE



This command is for the REACTOR_SIMULATOR (REACTOR) module.

The REACTOR workspace (along with the related POLY and GIBBS workspaces) and the simulated results from the SIMULATE command can be read by this command from a binary file where they must be saved with SAVE_WORKSPACE. The *.RCT file is not printable.

| Syntax | READ_WORKSPACE |
|---------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Options | <p>File name: The name of a saved *.RCT file where the REACTOR and POLY/GIBBS workspaces shall be read from must be specified. You do not need to type the extension if it is the default .RCT, otherwise type the whole *.RCT file name.</p> <p>An Open window displays if a file name is not given after the command or its path is incorrect, so that the path (in the Look in field) and File name can be specified. The Files of type (i.e. RCT) cannot be changed.</p> |

SAVE_WORKSPACES



This command is for the REACTOR_SIMULATOR (REACTOR) module.



The POLY module and Gibbs (GES) module also have a command with the same name.

The workspaces are saved to a file with this command. In the REACTOR workspace, all definitions of multi-stage steady-state reactor and its distribution coefficients are saved, together with the GIBBS and POLY workspaces.

After using this command, you can always return to the state when you issued the command by giving a READ command.

After saving the workspaces to a file, you can exit the software and at a later time READ the file and continue from the saved state.



START_SIMULATION automatically saves on the work file with the most lately specified name. To avoid destroying the simulated results, do not SAVE after a START_SIMULATE command is enforced, similar to that you should not use SAVE after a STEP or MAP command. You may append several results by START_SIMULATE without destroying the previous results but SAVE erases them all.


| Syntax | SAVE_WORKSPACES |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>File name</p> <p>A file name must be specified. The default extension of the RCT file is .RCT, while or any other extension as required.</p> |
| | <p>A Save window displays if a file name is not given after the command, so that the path (in the Save in field) and File name can be specified. The Files of type (i.e. RCT) cannot be changed. If there is already a file with the same file name under the directory a warning message displays. Click OK to overwrite the current REACTOR (and POLY3/GIBBS) workspaces onto the existing *.RCT file. Click Cancel to return to the REACTOR module. You can use the SAVE command with an unspecified name (i.e. through <code>SAVE , , ,</code> command-sequence) to save the REACTOR (and POLY3/GIBBS) workspaces.</p> |

START_SIMULATION



This command is for the REACTOR_SIMULATOR (REACTOR) module.

Start the reactor simulation, and list the results for all iterations. The output for each iteration consists of the conditions set in each segment, and you can also select some state variables to list. After each loop, the temperatures in all segments are listed.

| Syntax | START_SIMULATION |
|---------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Max number of loops /10/: <The max number of loops></p> <p>Give the max number of loops. The reactor simulation repeats until this loop number is reached.</p> |
| | <p>Output to screen or file /Screen/: <File name or return></p> <p>Decide on either listing simulation results on the screen (by pressing <Enter>) or saving them on an experimental file (with the default extension .EXP).</p> <div>  <p>The conditions in each segment are not saved in the file, only on the screen.</p> </div> |
| | <p>Output variables /T BP(\$)/: <Variable name(s)></p> <p>Specify the variable name(s) that is also listed on the screen together with the conditions in each segment, or in the output experimental file.</p> |

EXAMPLE OUTPUT

For a four-stage reactor, the output at a certain iteration may look like this:

```
H=-991745.1, P=100000, N(C)=2.8468936, N(N)=6.78399966E-4, N(O)=3.8171615,
N(SI)=1.77031
DEGREE OF FREEDOM 0
```

```

BP(GAS)=43.464341, BP(C1SI1_BETA)=25.175981, BP(C_S)=8.1588099,
BP(QUARTZ_S3)=68.193896
1.78803E+03
BP(GAS)=61.971213, BP(C1SI1_BETA)=38.144346, BP(QUARTZ_L)=66.230717 2.06569E+03
BP(GAS)=67.66262, BP(C1SI1_BETA)=35.480983, BP(QUARTZ_L)=58.219292
2.08691E+03
BP(GAS)=71.23129, BP(SI_L)=22.471787
2.20831E+03
H=-924751,87, P=100000, N(C)=2.0594558, N(N)=5.1799978E-4, N(O)=4.0142358,
N(SI)=2.7551438
DEGREE OF FREEDOM 0
BP(GAS)=43.464341, BP(C1SI1_BETA)=25.175981, BP(C_S)=8.1588098,
BP(QUARTZ_S3)=68.193896
1.78803E+03
BP(GAS)=61.971213, BP(C1SI1_BETA)=38.144346, BP(QUARTZ_L)=66.230717 2.06569E+03
BP(GAS)=67.66262, BP(C1SI1_BETA)=35.480983, BP(QUARTZ_L)=58.219292
2.08691E+03
BP(GAS)=71.23129, BP(SI_L)=22.471787
2.20831E+03
H=-813239., P=100000, N(C)=1.6592668, N(N)=3.59999988E-4, N(O)=3.7549293,
N(SI)=2.896635
DEGREE OF FREEDOM 0
BP(GAS)=43.464341, BP(C1SI1_BETA)=25.175981, BP(C_S)=8.1588098,
BP(QUARTZ_S3)=68.193896
1.78803E+03
BP(GAS)=61.971213, BP(C1SI1_BETA)=38.144346, BP(QUARTZ_L)=66.230717 2.06569E+03
BP(GAS)=67.66262, BP(C1SI1_BETA)=35.480983, BP(QUARTZ_L)=58.219292
2.08691E+03
BP(GAS)=71.23129, BP(SI_L)=22.471787
2.20831E+03
H=7374.6403, P=100000, N(C)=8.84911857E-1, N(N)=1.99999996E-4, N(O)=1.9379203,N
(SI)=1.853872
DEGREE OF FREEDOM 0
BP(GAS)=43.464341, BP(C1SI1_BETA)=25.175982, BP(C_S)=8.1588097,
BP(QUARTZ_S3)=68.193896
1.78803E+03

```

BP(GAS)=61.971213, BP(C1SI1_BETA)=38.144346, BP(QUARTZ_L)=66.230717 2.06569E+03
BP(GAS)=67.66262, BP(C1SI1_BETA)=35.480983, BP(QUARTZ_L)=58.219292
2.08691E+03
BP(GAS)=71.23129, BP(SI_L)=22.471787
2.20831E+03
10 1788.03 2065.69 2086.91 2208.31 0.00 0.00 0.00

POST Module Commands

The POST module (post-processor) is available from the these modules: POLY, TAB, BIN, TERN, POT, SCHEIL and POURBAIX.

► ["Using the POST Module" on page 101](#)

In this section:

| | |
|----------------------------------|-----|
| ADD_LABEL_TEXT | 352 |
| APPEND_EXPERIMENTAL_DATA | 353 |
| CHANGE_LEGEND | 354 |
| DUMP_DIAGRAM | 355 |
| ENTER_SYMBOL | 356 |
| FIND_LINE | 358 |
| LIST_DATA_TABLE | 358 |
| LIST_PLOT_SETTINGS | 359 |
| LIST_SYMBOLS | 359 |
| MAKE_EXPERIMENTAL_DATAFILE | 360 |
| MODIFY_LABEL_TEXT | 360 |
| PLOT_DIAGRAM | 361 |
| PRINT_DIAGRAM | 361 |
| QUICK_EXPERIMENTAL_PLOT | 362 |
| REINITIATE_PLOT_SETTINGS | 362 |
| RESTORE_PHASE_IN_PLOT | 362 |
| SELECT_PLOT | 362 |
| SET_AXIS_LENGTH | 363 |
| SET_AXIS_PLOT_STATUS | 363 |
| SET_AXIS_TEXT_STATUS | 363 |
| SET_AXIS_TYPE | 364 |

| | |
|-------------------------------|-----|
| SET_COLOR | 364 |
| SET_CORNER_TEXT | 365 |
| SET_DIAGRAM_AXIS | 366 |
| SET_DIAGRAM_TYPE | 368 |
| SET_FONT | 368 |
| SET_LABEL_CURVE_OPTION | 369 |
| SET_PLOT_FORMAT | 370 |
| SET_PLOT_OPTIONS | 370 |
| SET_PLOT_SIZE | 372 |
| SET_PREFIX_SCALING | 372 |
| SET_RASTER_STATUS | 372 |
| SET_REFERENCE_STATE | 372 |
| SET_SCALING_STATUS | 374 |
| SET_TIC_TYPE | 375 |
| SET_TIELINE_STATUS | 375 |
| SET_TITLE | 375 |
| SET_TRUE_MANUAL_SCALING | 376 |
| SUSPEND_PHASE_IN_PLOT | 376 |
| TABULATE | 376 |

ADD_LABEL_TEXT


Add a text to an area in a phase diagram or a property diagram. The label is written starting from the specified coordinates. Optionally, you can also let the program automatically add the text by first calculating an equilibrium state at the specified coordinates and then making a label out of the stable phase names.





The label texts and coordinates, either added by this command or modified with MODIFY_LABEL_TEXT (or manually edited in the **Console Results** window), are stored in the workspace, and these may later be saved onto an *.EXP file (with MAKE_EXPERIMENTAL_DATAFILE).



In some cases such an optional calculation for automatic phase region labeling may not work. It is not possible to automatically add labels for certain sets of axes, like entropy, enthalpy, pH, Eh, etc.

► ["Plot Labels " on page 234](#)

| Syntax | ADD_LABEL_TEXT |
|---------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Give X coordinate in axis units: <Value of the X coordinate></p> <p>Specify the value of the X coordinate where the label is to start.</p> |
| | <p>Give Y coordinate in axis units: <Value of the X coordinate></p> <div><p>The labels disappear if any axis is changed after wards.</p></div> <p>Specify the value of the Y coordinate where the label is to start.</p> |
| | <p>Automatic phase labels? /Y/:</p> <p>By default the program automatically calculates the equilibrium at the given coordinates and generates a label with the names of the stable phases. However, the automatic calculation works only for phase diagrams that are mapped with two axes in the POLY module, and sometimes it may not work correctly especially for complex heterogeneous interaction systems; in such cases, a message displays.</p> |
| | <p>Text: <Text for the label></p> <p>If you answer N enter text at the prompt. You can enter simple text, use LaTeX, rotate the text, as well as adjust the font size.</p> <p>LaTeX: You can use LaTeX commands to enter text and symbols. First enter the command followed by the expression or string, for example to display Al₂O₃ as subscripts:</p> <pre>\latex Mole-fraction Al_2O_3</pre> |

| Syntax | ADD_LABEL_TEXT |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p> For a list of supported LaTeX commands, see http://www2.ph.ed.ac.uk/snuggletex/documentation/math-mode.html.</p> <div>  <p>By default when using the LaTeX command, you are in math mode and Thermo-Calc automatically interprets the entered text as math. The above link uses the dollar sign (\$) in all the examples but this is NOT required. For example, if you enter $E=mc^2$ this is displayed including the \$ instead of the equation.</p> </div> <p> To add a mixture of plain text and equation text, you can exit math mode using the string <code>\textrm</code> followed by the text to display enclosed in curly brackets. For example <code>\latex \textrm{Mole-fraction }Al_2O_3</code> displays this label</p> <p style="text-align: center;"><code>Mole-fraction Al_2O_3</code></p> <p>Rotate the text: If you want to rotate the label, start a text string with the rotation command (which is case sensitive and must be in lower case letters) then enter the number of degrees to rotate the label. For example, to rotate the label 45 degrees enter:</p> <p><code>\rotation 45</code></p> <p>To rotate the text and use LaTeX, the rotation command must be used first. For example:</p> <p><code>\rotation 45 \latex Mole-fraction Al_2O_3</code></p> <p>Rotates the text 45° and includes subscripts in the title Mole-fraction Al₂O₃.</p> <p>Text size: <code>/.35/:</code> <Size for the label></p> <p>A smaller size of the text may be necessary to fit the label text into the diagram. A default size is given using the latest size in adding label texts, or .35 if the command is called for the first time. A recommended size is e.g. 0.25.</p> <p> These changes to plot labels can also be manually edited in the Console Results window.</p> |


APPEND_EXPERIMENTAL_DATA

Add experimental data and text onto a calculated diagram. This is done by placing the experimental data and text on a formatted textual file (always having an extension of EXP) that is prepared outside of Thermo-Calc software (Console Mode and Graphical Mode), according to the syntax of the DATAPLOT Graphical Language.

The picture generated from the data is superimposed on the ordinary graphical output from the postprocessor. Such an experimental data file (*.EXP) may be created by an ordinary textual editor.

Another important usage of this command is to superimpose plots from several independent calculations. For this purpose, there is a command `MAKE_EXPERIMENTAL_DATAFILE`, which dumps a calculated diagram on an EXP file according to the DATAPLOT syntax. With the aid of a normal text editor, many such files may be merged together. Remember that you can only have one prologue section on each such EXP file.

► *DATAPLOT User Guide* included with this documentation set.

| Syntax | APPEND_EXPERIMENTAL_DATA |
|---------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Use experimental data (Y or N) /N/:</p> <p>By default, no experimental data are plotted. Enter Y to use the data from an experimental data file in the next plot. An Open window displays to specify the name of the file with the experimental data.</p> |
| | <p>Prologue number: /0/: <Prologue number></p> <p>Select which prologue to use. In a prologue, you can, for example, give the scaling of an axis, the axis texts, and so on.</p> <div>  <p>By answering -1, a list of all prologues on the file is given; and by 0, no experimental data are appended.</p> </div> |
| | <p>Dataset number(s) /-1/: <Dataset number(s)></p> <p>Select from which dataset(s) data should be read. Several datasets may be given separated with commas or spaces. By answering -1, a list of all datasets on the file is given; and by 0, no experimental data are appended.</p> |

CHANGE_LEGEND

When there is a legend in the diagram you can append constitution and/or ordering descriptions to the phase name.




`LIST_EQUILIBRIUM` also displays `ORD` (ordered) or `DISORD` (disordered) (when available).



In some cases the legend only shows the phase name for a line when `SET_LABEL_CURVE_OPTION` is set to `F`.

| Syntax | CHANGE_LEGEND |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Set suffix for phase names in legend? (All, None, Constitution, Ordering)/None/:</p> <ul style="list-style-type: none"> None: the legend includes the standard information about the phases. |


| Syntax | CHANGE_LEGEND |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <ul style="list-style-type: none"> • All: the Constitution description and the Ordering description (when there is ordering) are also included. • Constitution: it is added to the standard description. • Ordering (when applicable): it is added to the standard description. |
| |  Also see "About Legend Styles" on page 236 for examples. |

DUMP_DIAGRAM

This is an alternative command used to create output. First use the PLOT_DIAGRAM command to send output to the Results window. Then you can save it to a file either using this command or right-click the diagram in the Results window and select Save as.



Similar to ["PRINT_DIAGRAM" on page 361](#), it does not matter what graphic device/printer is set up. The command can convert the diagram shown in the Results window to the selected format.

| Syntax | DUMP_DIAGRAM |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | Output format/: (jpg,ps,pdf,svg,emf,gif,png) /png/ |
| | <p>Enter a format or press <Enter> to accept the default (png).</p> <div>  <p>If you choose to enter the parameters and file name in one line (i.e. when you are entering the command), the Save window does not open as described below. For example, if you enter <code>dump_diagram png test</code> at the prompt, an image file called test.png is output to the same folder where the macro file is stored. If a file with the specified name already exists, you are prompted to overwrite the old file. You can alternatively add Y or N to the command string to specify whether to overwrite the file or not e.g. <code>dump_diagram png test y</code>.</p> </div> <p>A Save window opens if you have not specified a file name. Select a directory path and enter a File name. If a file with the specified name already exists, then you are prompted whether to overwrite the old file or not. The third argument of the command (Y) allows you to specify whether to overwrite the old file or not (N).</p> |



After the output is done, the temporarily set graphic device for conversion and printing is switched back to the one set by the command SET_PLOT_FORMAT, so that you can save the graph in file(s) using PLOT_DIAGRAM.

ENTER_SYMBOL



This command is for the POST module.



There are also a GES and POLY module commands with the same name.

Symbols are a useful feature of the POLY and POST modules to define quantities that are convenient. Symbols can be constants, variables, functions or tables.

Functions or tables (with defined functions as values) can be entered in the POST module after a stepping or mapping calculation, for purposes of plotting such entered functions or tables as axis variables.

Within the POLY module, symbols are normally defined prior to an equilibrium calculation (enforced by a C_E command), stepping calculation (enforced by the command STEP_WITH_OPTIONS) or mapping calculation (enforced by MAP). These can be entered after an equilibrium calculation; however, for defined functions, variable or tables, it requires using EVALUATE_FUNCTIONS before showing the corresponding values in the calculated equilibrium state.

The symbols entered in the POST module are not saved in the currently-loaded POLY3 workspaces. Therefore, if you want to apply such symbols in other similar calculations for the same defined system, you must use the ENTER_SYMBOL command prior to the STEPPING or MAPPING calculation in the POLY module.



See [example 44](#) for an example of using variables and functions.

Symbols are a useful feature modules to define quantities that are convenient. Symbols can be constants, variables, functions or tables.

| Syntax | ENTER_SYMBOL |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Constant, Variable, Function or Table? /Function/: <Keyword></p> <p>The Keyword can be specified as CONSTANT, VARIABLE, FUNCTION or TABLE.</p> <ul style="list-style-type: none">CONSTANTS can only be entered once and is a means of using a name for a numeric value. For example, the value of 1 atmosphere in Pascal can be denoted by P0 after the command ENTER_CONSTANT P0=101325. Defined constants can be used as values in condition assignments, for example, SET-COND P=P0.FUNCTIONS are expressions of state variables or other functions. These expressions are saved, and whenever a function value is requested all functions are evaluated. The reason for this is that they may depend on each other.VARIABLES are similar to functions because they can also be expressions of state variables. However, contrary to functions, they are only evaluated when they are entered or if they are explicitly named in an EVALUATE_FUNCTIONS command. It is possible to enter a variable with a new expression any time. This expression is evaluated directly and its value stored as the |

| Syntax | ENTER_SYMBOL |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>value of the variable. Defined variables can be used as values in the SET-CONDITION command.</p> <ul style="list-style-type: none"> • TABLES are used for listing results from the STEP or MAP commands. A table consists of a list of any number of state variables, functions or variables. Defined tables can also be used in the post-processor POST. <div data-bbox="350 478 402 531"> </div> <p>There is a special connection between tables and variables. If a variable is used in a table, it is evaluated for each line of the table in the TABULATE command or when the table is used in a plot.</p> |
| | <p>Name: <Name of the symbol></p> <p>Each symbol has a unique name that must start with a letter and can have maximum 8 characters.</p> <p>Legal characters include letters (either UPPER or lower case), digits and underscore <code>_</code>. Any other special character, such as parentheses (and), plus +, minus -, slash / or \, full stop (.), are illegal for symbol names.</p> <p>You can enter the symbol name and the value or function on the same line, these must be separated with an equal sign =, for example, <code>TC=T-273.15</code> or <code>T_C=T273.15</code> which stands for a definition of temperature in Celsius. Otherwise, these questions are asked.</p> <div data-bbox="350 968 402 1020"> </div> <p>For different types of symbol (constant, function, variable or table), the questions have different prompts.</p> |
| | <p>Function: <Definition for a function or variable></p> <p><i>Functions</i> and <i>variables</i> are evaluated from an expression of state variables or other functions, constants or variables. The expression is a FORTRAN-like expression and operators +, -, *, = and ** can be used (** only with integer powers).</p> <p>Unary functions like <code>LOG</code>, <code>LOG10</code>, <code>EXP</code>, <code>SIN</code>, <code>COS</code> and <code>ERF</code> can also be used. An expression can be continued on more than one line. An expression should be terminated by a semicolon (;) or an empty line (by pressing <Enter> at the next prompt).</p> <p>Examples of function expressions:</p> <ul style="list-style-type: none"> • <code>GM(LIQUID)</code>: The Gibbs energy of liquid per mole component • <code>H.T/4.184</code>: The heat capacity of the system in calories • <code>ACR(CR)/X(FCC,CR)</code>: The activity coefficient for Cr in FCC • <code>T-273.15</code>: The temperature in Celsius <p>&: <Continuation of the definition for the symbol></p> <p>The ampersand & means that you can continue to write the function on the new line if one line is not enough for the function. If you finish the function press <Enter> again.</p> |
| | <p>Value: <Value for a constant></p> <p>A <i>constant</i> can only be assigned a numeric value once.</p> |

| Syntax | ENTER_SYMBOL |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>Value or expression: <Value of expression for a variable></p> <p>A <i>variable</i> can be assigned a numeric value or an expression. An expression is evaluated immediately and discarded. Only the numeric value is kept. This gives a possibility to save a value between calculations with different conditions because all state variables and functions are evaluated for the new conditions.</p> |
| | <p>Variable(s): <Variable(s) in a table></p> <p>A <i>table</i> consists of a list of state variables or functions. One way to obtain results from a STEP command is through a table.</p> <p>Example:</p> <pre>ENTER TABLE K=T,X(LIQ,C),X(LIQ,CR),ACR(C)</pre> <p>Which means that the table called K contains four columns, i.e. the temperature, the mole fractions of C and Cr in the LIQUID phase, and the activity of C.</p> <p>To show the temperature in Celsius in a table, give the command ENTER_FUNCTION TC=T-273; and then use the symbol TC in the table.</p> <p>& <Continuation of the definition for the table></p> <p>The ampersand & means that you can continue to write the table on the new line if one line is not enough for the table. If you finish the table press <Enter> again.</p> |

FIND_LINE

Identifies various property curves on a plotted property diagram (after a stepping calculation); it also works well in find stable phase regions on a phase diagram (after a mapping calculation).

| Syntax | FIND_LINE |
|---------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>X coordinate /.484623611/: <Value of the X coordinate></p> <p>Specify the value of the X coordinate where you want to find the details of property curve (or phase region).</p> |
| | <p>Y coordinate /.5153737962/: <Value of the Y coordinate></p> <p>Specify the value of the Y coordinate where you want to find the details of property curve (or phase region).</p> <p>The POST module displays the identified property (for a property curve on a property diagram), or the identified stable phase-assemblage (for a phase region on a phase diagram).</p> |


LIST_DATA_TABLE



This is a POST module command.

This command is used for listing various properties (i.e. the Y-axis variable on a property diagram) that change with an independent variable (i.e. the X-axis variable on a property diagram), which have already been defined in the POST module (and often are plotted on the **Console Results** window), but only after a STEP calculation.

The listing output can be either on screen or in a spreadsheet file in the MS Excel format (under specified file name with the default file extension of XLS), which can be further edited or used for graphical handling by opening the file (using the MS-Excel program) outside of the Thermo-Calc software system.

| Syntax | LIST_DATA_TABLE |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Output to screen or file /Screen/: <File name or return ></p> <p>Specify a file name if you want to save on a spreadsheet file (in the MS Excel format, with the default extension of XLS) on which the already-defined properties on a property diagram (after a STEP calculation) is saved, or press <Enter> if want to see a simple textual table on screen (for the already-defined properties that change alone with an independent variable).</p> <p> This command only works for a property diagram after a stepping calculation but not for any phase diagram after a mapping calculation.</p> |

LIST_PLOT_SETTINGS



This is a POST module command.

| Syntax | LIST_PLOT_SETTINGS |
|--------|-------------------------------------------------------------------------------------------|
| | Lists the present values of most parameters specifying the type of diagram to be plotted. |

LIST_SYMBOLS



This command is for the POST module.



There is also a POLY module command with the same name.

Use this command to list the definitions for all constants, functions, variables and tables. In order to find the value of a function or variable, use SHOW_VALUE or EVALUATE_FUNCTIONS. A table is tabulated with the TABULATE command.

| Syntax | LIST_SYMBOLS |
|--------|----------------------------------------------------------------------------------------------------------------------------------|
| | The defined variables are listed up together with the defined functions, but variable names are followed by a percentage sign %. |

MAKE_EXPERIMENTAL_DATAFILE

Write the graphical information onto screen or a formatted text file (always having an extension of .EXP) using the DATAPLOT graphical format. In order to merge two or more diagrams from separate calculations, you can write them out on files with this command, and then add/edit them together with a normal text editor.




There is another type of experimental data file that is generated in Thermo-Calc when working with the PARROT module. For more information see "[Experimental Data Files \(*.POP, *.DOP\)](#)" on page 31.

| Syntax | MAKE_EXPERIMENTAL_DATAFILE |
|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | Output to screen or file /Screen/: <Name of a file or return> |
| Prompt | Specify the name of the desired file. Press <Enter> for a list. Otherwise enter a file name where the graphical information is written. The default file extension is EXP (for Windows) or exp (for Linux). |

MODIFY_LABEL_TEXT

Move a label created with the command ADD_LABEL_TEXT to another position, or replace its text with another one.

The label texts and the coordinates, either added by ADD_LABEL_TEXT command or modified by this command or manually edited on the Console Results window, are stored in the workspace, and can be saved onto an *.EXP file (through MAKE_EXPERIMENTAL_DATAFILE).

| Syntax | MODIFY_LABEL_TEXT |
|---------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | Which label to modify? /#/: <Number of the label> |
| Prompts | Before this prompt, all the labels created by the ADD_LABEL_TEXT command is listed with an identifying number. Specify the Number of the label you want to modify. The default one (#) is the last added label. |
| | New X coordinate: /xxx/: <New X position> Specify the New X position. The previous X coordinate is displayed. Press <Enter> to accept. |
| | New Y coordinate: /yyy/: <New Y position> Specify the New Y position. The previous Y coordinate is displayed. Press <Enter> to accept. |
| | New text /ABCDEFGH.../: <New labeling text> Specify the New labeling text. The previous text is displayed. Press <Enter> to accept. |
| | <div>The new label text must not be longer than the previous text.</div> |

PLOT_DIAGRAM


After you use the SET_PLOT_FORMAT command to define the default graphic device (the printer) you can use a PLOT_DIAGRAM command to either save the calculation output to a file or display the output in the Results window.



The diagram axes must be set first.

The functionality of this command is shared in two ways:

- in PLOT_DIAGRAM for normal screen display and file saving and
- *Windows OS*: If the device is not defined, you can alternatively use PRINT_DIAGRAM for a hard copy.

| Syntax | PLOT_DIAGRAM |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | Output to screen or file /Screen/: <Name of a file or return for screen> Specify the name of the file |
| | <div> For Linux users, the prompt is PLOTFILE /SCREEN/).</div> <p>A file with a proper extension for the selected graphic format (set by SET_PLOT_FORMAT) is saved under the current working directory. If no extension is given in the file name, the default extension e.g. ps for Postscript portrait/landscape modes, P7 or p7 for HPGL landscape, P8 or p8 for HPGL portrait, etc.) is automatically given to the file name.</p> <p>If the default device is set (SET_PLOT_FORMAT), press <Enter> to plot the diagram on the screen in the Console Results window or give a file name to save it.</p> |

PRINT_DIAGRAM



["Saving and Printing the Output in Console Mode" on page 102](#)

First use PLOT_DIAGRAM to create a diagram that displays in the **Console Results** window. Then after entering the PRINT_DIAGRAM command, the **Print** window opens where you can choose additional settings for a hard copy of the diagram.



PRINT_DIAGRAM functions in the same way as in the **Console Results** window where you can right-click a diagram and choose **Print**.

QUICK_EXPERIMENTAL_PLOT

This is similar to APPEND_EXPERIMENTAL_DATA but can be used when there is no graphical information to be plotted in the POLY3 workspace. It defines a pair of axes, sets the axis labels to X and Y, and scales both X- and Y-axes between 0.0 and 1.0 unless a prologue is read from the DATAPLOT (*.EXP) data file.

► ["Plotting Experimental Data Files" on page 4](#) in the *DATPLOT User Guide* included with this documentation set.

| Syntax | QUICK_EXPERIMENTAL_PLOT |
|---------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Prologue number: /0/: <Prologue number></p> <p>An Open window displays. Select the prologue to use. In a prologue, you can, for example, give the scaling of an axis, the axis texts, and so on. By answering -1, a list of all prologues on the file is given; and with 0, no experimental data are appended.</p> |
| | <p>Dataset number(s) /-1/: <Dataset number(s)></p> <p>Select from which dataset(s) data should be read. Several datasets may be given separated with commas or spaces. By answering -1, a list of all datasets on the file is given; and with 0, no experimental data are appended.</p> |

REINITIATE_PLOT_SETTINGS

The REINITIATE_PLOT_SETTINGS command gives default values to all parameters describing the diagram. All plot settings made in the POST module are deleted, and it returns to the initial settings when the POST module is entered.

RESTORE_PHASE_IN_PLOT

Restores a phase previously suspended from the plot with SUSPEND_PHASE_IN_PLOT. It works only after at least one phase is suspended.

| Syntax | RESTORE_PHASE_IN_PLOT |
|--------|----------------------------------------------------------------------------------------------|
| Prompt | <p>Phase name: <Name of a phase></p> <p>Give the name of the phase to be restored.</p> |

SELECT_PLOT

Select a plot (diagram) within the current **Results** tab in the **Console Results** window.

| Syntax | SELECT_PLOT |
|--------|--------------|
| Prompt | Plot <N/New> |

| | |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | SELECT_PLOT |
| | <p>Where N is a positive integer. Enter the number of the plot that is selected in the Console Results window (in the currently selected Results tab). If a plot with that number does not exist, it is created.</p> <p>The default parameter value is NEW. If this is entered, then a new plot is created. Create a new plot can also be done by pressing <Ctrl+Shift+T>.</p> |

SET_AXIS_LENGTH

Change the real length of an axis in inches. The default number of tic-marks on an axis is 10 when the relative length is 1. The number and units per tic-mark must be a multiple of 1, 2 or 5 to obtain a reasonable scaling of an axis.

| | |
|---------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | SET_AXIS_LENGTH |
| Prompts | <p>Axis (X, Y or Z): <Name of an axis></p> <p>Specify which axis to set the length.</p> |
| | <p>Axis length /11.5/: <New relative axis length></p> <p>Specify the new real axis length in inches. The relative length 1 corresponds to 10 tic-marks on the axis.</p> |

SET_AXIS_PLOT_STATUS

Specify whether the axis title texts and axis label texts are to be plotted or not on a diagram. It does not work for the axis lines and tic-marks. If you want to plot a diagram without tic-marks, use SET_TIC_TYPE first.

This can be used to merge different diagrams on a pen-plotter or to obtain the diagram faster. The default status is that all the set axes are to be plotted.

| | |
|--------|----------------------------------|
| Syntax | SET_AXIS_PLOT_STATUS |
| Prompt | Axis plot (Y or N) /Y/: (Y or N) |

SET_AXIS_TEXT_STATUS

Change the axis text from the automatic text given by the axis specification to a text.

► ["ADD_LABEL_TEXT" on page 352](#)

| | |
|---------|---------------------------------------------------------------------------------------------------|
| Syntax | SET_AXIS_TEXT_STATUS |
| Prompts | <p>Axis (X, Y or Z): <Name of an axis></p> <p>Specify which axis text status to change.</p> |

| Syntax | SET_AXIS_TEXT_STATUS |
|--------|-------------------------------------------------------------------------------------------------------------------------|
| | Automatic axis text (Y or N) /N/: Specify if automatic axis text is to be used. |
| | Axis text: <Enter axis text> You can enter simple text, use LaTeX, rotate the text, as well as adjust the font size. |

SET_AXIS_TYPE

Change the axis type among linear, logarithmic and inverse axis.

| Syntax | SET_AXIS_TYPE |
|---------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | Axis (X, Y or Z): <Name of an axis> Specify which axis to change the axis type. |
| | Axis type /Linear/: <New axis type> Specify which new axis type to set. Select <code>Linear</code> (default), <code>Logarithmic</code> or <code>Inverse</code> . Only the three first characters are relevant. |

SET_COLOR


Some devices support colours or line thickness. With this command, select different colors or line types on some types of information on a diagram.



This command can fail if a chosen device does not support colors or line thickness.

This command gives four sequential prompts (i.e. text and axis, invariant equilibria, tie-lines, and all other lines), with the keyword and default option (both listed below). Depending on if the switched-on graphic device (by SET_PLOT_FORMAT) supports colors or line types, the POST automatically switches on the appropriate Keyword.

| Syntax | SET_COLOR |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | Text and axis keyword /Default option/ <Return or new option> Invariant equilibria keyword /Default option/: <Return or new option> Tie-lines color keyword /Default option/: <Return or new option> Keyword of all other lines /Default option/: <Return or new option> This is usually for the solubility lines. |

| Syntax | SET_COLOR |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| |  <p>The <code>Keyword</code> is either <code>Color</code> or <code>LineType</code>, depending on if color or line type is supported by the switched-on graphic device (by <code>SET_PLOT_FORMAT</code>); the POST module <i>automatically</i> switches on the appropriate <code>Keyword</code>.</p> |

COLOR OPTIONS

The options for `Color` are:

| | | | |
|----------------------------------------|---------|------------|------------|
| BACKGROUND | BLUE | PURPLE | GRAY |
| FOREGROUND (default) | YELLOW | GOLD4 | ORANGERED3 |
| RED (default for invariant equilibria) | MAGENTA | TURQUOISE4 | MAROON |
| GREEN (default for tie lines) | CYAN | PINK | PLUM |
| | SIENNA | OLIVEDRAB | SEAGREEN |
| | ORANGE1 | CORAL1 | USERDEF |

LINE TYPE OPTIONS

The options for `LineType` are:

| | |
|------------------|-----------------------------------------------|
| INVISIBLE | VERY_THICK (default for invariant equilibria) |
| NORMAL (default) | THIN (default for tie lines) |
| THICK | VERY_THIN |
| DASHED | DOTTED |

SET_CORNER_TEXT

Adds text to the corners on a plotted diagram. Normally, you can write such texts as a subtitle.

The primary database (not the appended ones) used in calculations and the calculated conditions are automatically plotted at the upper-left corner as a part of the header on all plotted diagram. Unless the plotting option `WRITE CONDITIONS` is switched off by the command `SET_PLOT_OPTIONS`, the calculated conditions are always written on plotted diagrams; and only when the plotting option `PLOT HEADER` is switched off by the command `SET_PLOT_OPTIONS`, the used database also always appear. Under such circumstance, avoid writing texts at the `UPPER_LEFT` corners.

| Syntax | SET_CORNER_TEXT |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Corner/Lower_Left/: <Return or new option></p> <p>Choose an option:</p> <ul style="list-style-type: none"> • LOWER_LEFT • UPPER_LEFT • UPPER_RIGHT • LOWER_RIGHT • TOP_OF_TRIANGLE |
| | <p>Text: <Texts as a subtitle or a note></p> <p>Write the texts that are to be written on the specified diagram corner.</p> |

SET_DIAGRAM_AXIS

Specify an axis variable for a plot or a listing. To be able to plot a diagram, at least two axis variables (X and Y) must be specified. In Console Mode, three axes (X, Y, and Z) can be specified for a diagram.



The axis variables in the plot can be different from the number of axis used for the mapping.

If you want to plot a phase diagram with tie-lines in the plane after a MAP calculation, then the composition axis must be `mole-fraction` or `weight-fraction`, or `mole-percent` or `weight-percent` of one specific component. You must not use the stable variable `x(comp)` or `w(comp)` even if that is what you used when calculating the diagram, because that only gives one side of the two-phase region. It may be sufficient to indicate that mole-fraction is the same as the stable variable `x(*, comp)`, and weight-fraction is the same as the stable variable `w(*, comp)`.

If you plot a phase diagram where the tie-lines are not in the plane after a MAP calculation, then `mole-fraction` and `x(comp)` are identical.

When you plot a property diagram after a STEP calculation and want a composition axis variable, you should normally use `x(comp)` and not mole-fraction.

The axis must have exactly the same number of columns, or one axis must have one column. In the first case the columns are plotted matching them one by one; in the latter all columns on one axis is plotted against the single column. For example, you can have the temperature on one axis and the amount of each phase on the other. The amount of each phase is the state variable `NP(*)` in mole fraction or `BPW(*)` for mass fractions of phases.

Automatic diagram axis: The POST module can set automatic diagram axis identical to those used in the MAP command.

If the state variable $x(\text{comp})$ is used in a MAP calculation, then mole-fraction of the component is used as diagram axis; if a potential or some other state variables are used, then that is used as a diagram axis.

After a STEP calculation, automatic diagram axis is not set as there is only one axis used in the calculation.


| Syntax | SET_DIAGRAM_AXIS |
|---------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>Axis (X, Y or Z): <Axis name></p> <p>Specify which axis (X or Y or Z) to set with a variable.</p> |
| Prompts | <p>Variable type: <Variable name></p> <p>Specify a variable for the chosen axis here.</p> <p>The valid variables are:</p> <ul style="list-style-type: none"> • TEMPERATURE-CELSIUS as temperature in °C • TEMPERATURE as temperature in K • PRESSURE as pressure in Pa • ACTIVITY for a component • LNACTIVITY for a component [ln(ACR(component))] • MOLE-FRACTION for a component • MOLE-PERCENT for a component • WEIGHT-FRACTION for a component • WEIGHT-PERCENT for a component • ENTHALPY as enthalpy in J/mol • ENTROPY as entropy in J/mol/K • NONE to clear the axis • Any valid state variable including those with wildcards, e.g. NP(*) or x(*,component). Due to the use of wildcard * in such a state variable, the program asks for a column number. • Any entered function or variable. • Any entered table. |
| | <p>If you specify an entered table as the variable, then you are given these prompts:</p> <p>For component: <Component name></p> <p>When an activity, mole or weight fraction or percent of a component shall be plotted, the component name must be supplied here.</p> |
| | <p>Column number: <Column number(s)></p> <p>Specify the column number(s) in the chosen table that are to be plotted onto the earlier specified</p> |

| Syntax | SET_DIAGRAM_AXIS |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>axis. For example:</p> <ul style="list-style-type: none"> • 1 for column 1 • 2,3 for columns 2 and 3 • 2,3 >5 for column 2,3 and all columns above column 5 • * for all columns |

SET_DIAGRAM_TYPE

Choose the diagram type as perpendicular plot or triangular plot (Gibbs triangle, especially for ternary systems). The default is with a perpendicular axes.

For phase diagrams of ternary or pseudo-ternary systems, it is usually need to plot isothermal sections as triangular grams. If desired, all lines outside the region limited by a line joining the end points of the X- and Y-axis is removed.

| Syntax | SET_DIAGRAM_TYPE |
|---------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>Triangular diagram (Y or N) /N/:</p> <p>The default is to set a perpendicular axis. Perpendicular diagrams have (almost) the same scaling on both axes.</p> |
| Prompts | <p>Create tetrahedron WRML file (Y or N) /N/:</p> <p> The 3D plotting in Console Mode does not work. Enter Y to specify a triangular plot instead.</p> |
| | <p>Plot 3rd axis (Y or N) /N/:</p> <p>If a triangular plot is selected, enter Y to specify a 3rd axis and to connect (and plot) the end points of the X- and Y-axes.</p> |
| | <p>Clip along 3rd axis (Y or N) /N/:</p> <p>If a triangular plot is selected, enter Y so that all lines outside the region limited by a line joining the end points of the X- and Y-axis are removed.</p> |

SET_FONT

Select the font to use for labels and numbers when plotting the diagram under the currently selected graphic device (SET_PLOT_FORMAT). For some devices there may be other fonts available and these are selected by SET_PLOT_FORMAT.

| Syntax | SET_FONT |
|---------|-----------------------------|
| Prompts | Select font number /1/: <#> |


| Syntax | SET_FONT |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | Specify an available font number # as the default font for the current graphic device, or accept the font number 1 by pressing <Enter>. By typing a question mark ? here, the program lists the available fonts under the currently selected graphic device. |
| | Font size /.34/: <##> The size of the chosen font is specified. A value around 0.34 is recommended. |

SET_LABEL_CURVE_OPTION

Identify the curves drawn in the post-processor by marking each curve with a digit and then list the meaning of these digits beside the plot.



The number of digits can be quite large in some cases. If so, use SET_FONT and reduce the font size; usually, 0.2 is sufficient.

| Syntax | SET_LABEL_CURVE_OPTION |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | Curve label option (A, B, C, D, E, F OR N) /A/: <Option> |
| | <p>The options:</p> <ul style="list-style-type: none"> • A: List stable phases along line • B: As A but curves with same fixed phase have same number • C: List axis quantities • D: As C but curves with same quantities have same number • E: As B with changing colors • F: As D with changing colors • N: No labels <p>This question is rather cryptic but usually the option B or E is good for phase diagrams (after a MAP command) and option D or F for property diagrams (after a STEP command). Those interested can try out the option A and C by themselves.</p> <div>  <p>Option B or E lists the fixed phases along each curve, whereas option D or F gives the axis variables used along each curve. E provides varied colors for different stable-phase curves on phase diagrams (after a MAP command); F provides varied colors for different property curves on property diagrams (after a STEP command). The option N (NONE) disables all curve labels and lists.</p> </div> <p>If, for example, you use T (temperature in K) as the variable axis in a STEP command and then plot the amount of stable phases (with SET_DIAGRAM_AXIS Y NP(*)) on the Y-axis versus T-C on the X-axis, then the list may have lines like:</p> <pre>1: T-273.15, NP(LIQUID)</pre> |

| Syntax | SET_LABEL_CURVE_OPTION |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>2: T-273.15, NP(FCC_A1)</p> <p>This means that for curve 1 the X-axis is T-273.15 (the same for all curves, of course) and NP (LIQUID) on the Y-axis. Curve 2 has the same X-axis but NP(FCC_A1) on the Y-axis.</p> |

SET_PLOT_FORMAT

Set the format of the graphical output to different graphical devices. The default graphic device is normally for screen output (number 22 - TCUNITE Driver). Legacy devices can still be used (1 for Windows and 9 for XWindow for Linux). This default graphic device value may also be altered with SET_PLOT_ENVIRONMENT in the system monitor or by your TC.INI file.

| Syntax | SET_PLOT_FORMAT |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <p>Graphic device number /#/: <Number of the device></p> <p>Specify a graphic device number. Depending on the hardware, different plot formats (graphic devices) may be available. These are listed online by giving a question mark ?.</p> <p>For some formats there can be additional sub-prompts (Y or N) about the available fonts being used for the chosen format. Also enter Y for further specifications, e.g. font type and size.</p> |

SET_PLOT_OPTIONS

You are prompted for and can toggle on (Y) or off (N) the plotting of some options on all subsequently generated diagrams.

For the `Always initiate POST on re-entering` prompt, the default is Y which implies that the POST module automatically reinitiates whenever the POLY3 workspace is changed upon re-entering. If answered N the same diagram axis variables are kept even if the workspaces in the POLY module are read from or written to a *.POLY3 file. The N answer is useful when there are several sets of *.POLY3 files with the same calculation but for different sets of model parameters.

For the `Always solid line` prompt, the default answer is N which means that the POST module plots solid lines for stable phases but dashed lines for metastable phases. This is normally for plotting property diagram after a STEPPING calculation; however, when there is a metastable extrapolation in a phase region on a phase diagram after a MAPPING calculation, this is also enforced. When the alternative answer Y is chosen, all the lines are always plotted in solid lines.

| Syntax | SET_PLOT_OPTIONS |
|---------|----------------------------------------------------------------------------------------|
| Prompts | <p>Plot header /Y/:</p> <p>Toggle the plotting of the header text above a diagram.</p> |

| Syntax | SET_PLOT_OPTIONS |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>Plot logo /Y/:</p> <p>Toggle the plotting of the Thermo-Calc logo at the lower-left corner of a diagram.</p> |
| | <p>Plot footer /Y/:</p> <p>Toggle the plotting of the footer identifier text at the right margin of a diagram.</p> |
| | <p>White-Contoured-PS-CHARS /Y/:</p> <p>By default, the PostScript characters are written as a white contoured status.</p> |
| | <p>Plot remote exponent(s) /Y/:</p> <p>By default the remote exponent on the axis is plotted.</p> |
| | <p>Plot symbols at node points /0/: <#></p> <p>This makes it possible to plot symbols at the node points on plotted lines on a diagram.</p> |
| | <p>Symbol size /.1/: <.#></p> <p>Set the size of symbols which are plotted at the node points.</p> |
| | <p>Write condition? /Y/:</p> <p>By default, the initial equilibrium conditions for the current calculations are automatically plotted at the upper-left corner as a part of the header. If you enter N, the calculated conditions are not included on a plotted diagram.</p> |
| | <p>Write database name? /Y/:</p> <p>By default, the primary database (not appended ones) used in the current calculations are plotted at the upper-left corner as a part of the header. If you enter N, the database name is not included on a plotted diagram.</p> |
| | <p>Always initiate POST on re-entering: /Y/:</p> <p>By default the POST module automatically reinitiates whenever the POLY3 workspaces are changed upon re-entering.</p> <p>If you enter N, the same diagram axis variables are kept even if the workspaces in the POLY module is read from or written to a *.POLY3 file. This can be useful when there are several sets of *.POLY3 files with the same calculation but for different set of model parameters.</p> |
| | <p>Always solid line: /N/:</p> <p>By default the POST module plots solid lines for stable phases and dashed lines for metastable phases. This is normally for plotting property diagrams after a STEPPING calculation. However, when there is a metastable extrapolation in a phase region on a phase diagram after a MAPPING calculation, this is also enforced. Enter Y to always plot solid lines in this case, for example.</p> |

SET_PLOT_SIZE

Change the size of the diagram by specifying a global plot size (as a relative scaling factor). The default value of the relative scaling factor is 1, while the real size of the plotted diagram depends on what output device is chosen with SET_PLOT_FORMAT. The default plot size (corresponding to the default global plot size 1) is adjusted to the chosen device.

| Syntax | SET_PLOT_SIZE |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | Global plot size /1/: <Relative scaling factor> |
| Prompt | Enter the relative scaling factor as a numerical number (e.g. 0.5, 0.8, 1.0, 1.5, etc.). By pressing <Enter>, the default relative scaling factor (1) is accepted. |

SET_PREFIX_SCALING

Specify on which axis is to have a prefix scaling then set the scaling of remote exponents with certain powers.

| Syntax | SET_PREFIX_SCALING |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | Axis (X, Y or Z): <Name of an axis> |
| Prompt | Specify which axis is to have a prefix scaling. |
| | Use prefix scaling /Y/: (Y or N or #) <ul style="list-style-type: none">• NO switches off its action.• YES arranges the prefix scaling so that the axis scaling is done with the remote exponents being powers of three, i.e. ..., -6, -3, 0, 3, 6, The default is 3.• # is an integer number that sets the remote exponents as being powers of # (as the powers for the remote exponents). |

SET_RASTER_STATUS

Plot a raster (i.e. with gridlines on both axis directions) in the diagram.

| Syntax | SET_RASTER_STATUS |
|--------|-----------------------------------------------------------------------|
| | Raster plot (Y or N) /N/: |
| Prompt | By default no raster is plotted. Enter Y to plot using a raster plot. |

SET_REFERENCE_STATE



This command is available for the POLY, ED-EXP and POST modules.

The reference state for a component is important when calculating activities, chemical potentials and enthalpies and is determined by the database being used. For each component the data must be referred to a selected phase, temperature and pressure, i.e. the reference state.





All data in all phases where this component dissolves must use the same reference state. However, different databases can use different reference states for the same element/component. It is important to be careful when combining data obtained from different databases.

By default, activities, chemical potentials and so forth are computed relative to the reference state used by the database. If the reference state in the database is not suitable for your purposes, use this command to set the reference state for a component using `SER`, i.e. the Stable Element Reference (which is usually set as default for a major component in alloys dominated by the component). In such cases, the temperature and pressure for the reference state is not needed.

In order to specify conditions in the specific reference state, you can append an `R` to the state variables. Thus, `AC` is the activity (of a system component or of a species in a phase) with respect to the default reference state, and `ACR` is the activity with respect to the selected reference state; `MU` is the chemical potential of a system component with respect to the default reference state, and `MUR` stands for the chemical potential with respect to the selected reference state. The `AC` and `ACR` variables, for both components in a system and species in a phase, can be specified in natural logarithm, e.g. `LNAC(Fe)`, `LNACR(C)`, `LNAC(O2,GAS)`, `LNACR(O2,GAS)`.

For the POST module, and after calculating with the `STEP_WITH_OPTIONS` or `MAP` commands, the reference state for a component can also be changed to plot various properties of the component in the entire system or in a specific phase. Then you can set the diagram axes as the chemical potential or activity quantities with the `R` suffix, i.e. `MUR(comp)`, `MUR(comp,ph)`, `ACR(comp)`, `ACR(comp,ph)` or the common logarithms [e.g. `LNACR(comp,ph)`].

| Syntax | SET_REFERENCE_STATE |
|---------|--------------------------------------------------------------------|
| Prompts | Component: <Name of the component> |
| | The name of the component must be given. |
| | Reference phase: <Name of a phase used as the new reference state> |
| | Enter the Name of a phase for the system. |

| Syntax | SET_REFERENCE_STATE |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| |  <p>For a phase to be usable as a reference for a component, the component needs to have the same composition as an end member of the phase. The reference state is an end member of a phase. The selection of the end member associated with the reference state is only performed once this command is executed.</p> <p>If a component has the same composition as several end members of the chosen reference phase, then the end member that is selected at the specified temperature and pressure will have the lowest Gibbs energy.</p> <p>The following are example using temperature. Pressure is used in the same way:</p> <ul style="list-style-type: none"> • In the Fe-C system, BCC can be a reference state for Fe but not for C since BCC can exist as pure Fe but cannot exist as pure C. • If GAS is chosen as the reference phase of component O at such a high temperature that O1 has the lowest energy, then O1 remains the reference state even at calculations performed at lower temperatures where O2 has a lower energy than O1. • Setting the reference state for component O as gas (one sublattice) with constituents O1, O2 and O3 results in O2 being the reference state if, at the present temperature, pure O2 has the lowest energy of O1, O2 and O3. If the reference state is set above a critical higher temperature, then O1 has the lowest energy and consequently becomes the reference state. |
| | <p>Temperature /*/: <Temperature for the reference state></p> <p>Select the Temperature (in K) for the reference state. The wildcard value * means the current temperature is used at the time of evaluation of the reference energy for the calculation.</p>  <p>The temperature set with this command does not affect the temperature used when evaluating the energy of the reference state during the end member selection process.</p> |
| | <p>Pressure /1E5/: <Pressure for the reference state></p> <p>Select the Pressure (in Pa) for the reference state. The wildcard value * means the current pressure is used for evaluating the reference energy at the time of calculation.</p> |
| | <p>EXAMPLES</p> <pre> S-R-S Fe SER S-R-S Cr FCC * 100000 S-R-S H2O AQUEOUS * 100000 S-R-S ZE REF_ELECTRODE * 100000 </pre> |

SET_SCALING_STATUS

When an axis variable is selected by SET_DIAGRAM_AXIS, the scaling status for the axis is always set to automatic scaling. By this command, choose between manual or automatic scaling on a specified axis. If manual scaling is chosen, specify a minimum and a maximum

value. Manual scaling can be used to magnify interesting parts of a diagram.

| Syntax | SET_SCALING_STATUS |
|---------|------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | Axis (X, Y or Z): <Name of an axis> Specify which axis that you want to set the scaling status. |
| | Automatic scaling (Y or N) /N/: The default is manual scaling. Enter Y for automatic scaling (N). For manual scaling specify the Min and Max values. |
| | Min value: <Minimum value> The minimum value at the start point of the specified axis. |
| | Max value: <Maximum value> The maximum value at the end point of the specified axis. |

SET_TIC_TYPE

Change the drawing of the axis tics. You may alter the placement of tic marks on the axis, e.g. inside or outside or no tic marks. The size of tic marks cannot be altered by this command, but these are adjusted based on the selected graphic device and the defined relative scaling factor (global plot size).

| Syntax | SET_TIC_TYPE |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | TIC Type /1/: <1 or -1 or 0> The tic type 1 is default, i.e. the tics are drawn outside the diagram. -1 means that the tics are inside the diagram and 0 means no tics. |

SET_TIELINE_STATUS


If the tie-lines are in the plane of the calculation, you can select to plot the tie-lines in two-phase fields with this command.

| Syntax | SET_TIELINE_STATUS |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | Plotting every tie-line no. /0/: <Number of tie-lines> The tie-lines plotted are not equally spaced by the graphics software. Instead, you can select to plot a subset of the calculated tie-lines, i.e. every one (1), every second (2), every three (3), etc. By accepting the default value 0, no tie-line is plotted. |

SET_TITLE

Specify a title that displays on all listed tables and plotted diagrams from the POST module.

► ["ADD_LABEL_TEXT" on page 352](#)

| Syntax | SET_TITLE |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <div>Title</div> <div>Enter the title you want to appear on all tabulation or graphic outputs.</div> <div> There is a maximum length of about 60 characters for the title. You can enter simple text, use LaTeX, rotate the text, as well as adjust the font size.</div> |

SET_TRUE_MANUAL_SCALING

The tic-marks on the axes are normally placed in even intervals using the whole axis length. The scaling routine adjusts the given minimum and maximum values slightly to accomplish this. If such an automatic adjustment behaviour is unwanted, it can be avoided by using this command (followed by a message showing the TRUE MANUAL SCALING set for a specific axis).

The command works like a toggle. To reset the automatic scaling behaviour, repeat the command a second time for that specific axis (followed by a message saying the SEMI_MANUAL SCALING set for the specific axis).

| Syntax | SET_TRUE_MANUAL_SCALING |
|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompt | <div>Axis (X, Y or Z): <Name of an axis></div> <div>Specify which axis (X or Y or Z) you want to toggle between automatic adjustments or avoid the adjustment of the given maximum and minimum values.</div> |

SUSPEND_PHASE_IN_PLOT

Specify that lines originating from the presence of a certain phase shall not be plotted on a diagram. If you want to bring the suspended phase back to the diagram, use RESTORE_PHASE_IN_PLOT.

| Syntax | SUSPEND_PHASE_IN_PLOT |
|--------|---------------------------------------------------------------------------------------------------------------------------|
| Prompt | <div>Phase name: <Name of a phase></div> <div>Specify the name of the phase to be suspended from the diagram.</div> |

TABULATE



This command is available for a table entered in either the POLY or POST module.

For any entered table, this command gives a table of values from equilibria calculated with a STEP command.



Unlike the TAB module's command (also called TABULATE) it is not possible to plot columns from the tabulated tables. For this use normal POST commands.

| Syntax | TABULATE |
|---------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <p>Name: <Name of a table entered in either POLY or POST></p> <p>Specify a table name that is entered in either the POLY or POST module.</p> |
| | <p>Output on screen or file /Screen/:</p> <p>Specify a file name if you want to save on a file the table values along the defined STEP calculation, or press <Enter> if want to see the table values displayed.</p> |

Parameters, Functions and Variables

This section is applicable to both Console Mode and Graphical Mode with respect to understanding the format these are to be written in for Thermo-Calc to use the parameter, function or variable. However, many of the sections are specific to Console Mode where the explicit use of these terms is more often used.



To learn about using variables and functions: For Graphical Mode, see "[T 07: User-Defined Functions](#)" on page 256 and for Console Mode, see [example 44](#) .

In this section:

| | |
|-----------------------------|-----|
| Specifying Parameters | 379 |
|-----------------------------|-----|

Specifying Parameters



This section or topic is specific to Console Mode.

Running a command typically requires that several parameter values are specified, which can be done directly in the command line after the command name. For example, to set an axis variable for a stepping or mapping operation, enter:

```
SET_AXIS_VARIABLE 1 X(FCC,FE) 0 0.89 0.025
```

You can also use SET_AXIS_VARIABLE and press <Enter>. At the command line prompt, you then specify the parameters one at a time.

On all command lines, you can enter a question mark (?) for help. For some parameters, enter two question marks (??) for more detailed information.

DEFAULT PARAMETERS VALUES

When you are requested to specify a parameter, Thermo-Calc usually suggests an appropriate default value, which is displayed at the prompt between two slash signs (/). For example, this prompt means the default answer is `TERMINAL`:

```
OUTPUT FILE /TERMINAL/:
```

Press <Enter> to accept the default.

If you specify some parameters directly after the command name, then you can still choose to accept default values for some parameters.

To accept the default value for a parameter, type a comma (,) instead of a value for that parameter. For the comma to be interpreted correctly, type a blank space on each side of the comma. However, if you accept the default values for several parameters that follow each other, then the commas can be typed in without blank spaces separating them: (, , ,) is interpreted in the same way as (, , ,).

For some commands and parameters, Thermo-Calc treats the values previously assigned as default values if the command is used again. For example, if the first stepping or mapping axis variable is specified as:

```
SET_AXIS_VARIABLE 1 X(FCC,FE) 0 0.89 0.025
```

Then if you want to change a parameter value for this axis variable, type:

```
SET_AXIS_VARIABLE 1 , 0.1 , , ,
```

This changes the minimum value from 0 to 0.1 at which a stepping or mapping operation halts. The other parameter values remain the same. Consequently, what is typed is equivalent to:

```
SET_AXIS_VARIABLE 1 X(FCC,FE) 0.1 0.89 0.025
```

Thermodynamic Variables and Units

The following topics are about the different thermodynamic variables recognized by Thermo-Calc. The topics have information about how to define new derived variables and functions and how to express thermodynamic variables in non-default units.



The POLY module only recognizes default units, which are SI units.

In this section:

About Operators and Functions

Sometimes you need to specify functions when setting up a system. For example, to make global conditions vary as a function of time.

The following operators can be used in writing functions. Use a semi-colon (;) to mark the end of a function.

Available Operators for Writing Functions

| Operator | Description |
|-------------------------|-----------------------------------------------------------------------------------------|
| +, -, *, / | Addition, subtraction, multiplication, division |
| ** | Exponentiation, raising one quantity to the power of another, e.g. x^2 . |
| ABS() | Absolute value |
| ERF(X) | Error function |
| EXP(X) | Exponential |
| LOG(X) | Natural logarithm |
| LOG10(X) | Base 10 logarithm |
| SIGN(X) | Sign function SIGN(X) is -1 when $X < 0$, is 0 when $X = 0$ and is 1 when $X > 0$. |
| SIN(X), COS(X), ATAN(X) | Sinus, cosinus and arctangent |
| SQRT(X) | Square root |

Thermodynamic Variables

There are different thermodynamic variables in Thermo-Calc. Some are *state variables*, for example temperature, pressure and mole fraction. These characterize the equilibrium state of a system. You set them when you define your system in the POLY module before performing a calculation. They are also used in other modules such as DATA, GIBBS and PARROT. State variables that involve components can be used for the defined components, but not for any species. (To define new components in a defined system, use ["DEFINE COMPONENTS" on page 160](#)).

Other useful thermodynamic variables are derived from state variables with a mathematical function. Some derived variables are pre-defined by Thermo-Calc, such as normalized energetic and compositional extensive state variables for example. You use these by appending various normalizing suffixes to abbreviations that are associated with the state variables.

Thermodynamic variables can also be divided into extensive variables and intensive variables. An extensive variable is a variable whose value depends on the size of the system, whereas an intensive variable is a variable whose value is independent of system size.

More information about thermodynamic variables is available in the online help in Thermo-Calc Console Mode. Use the command ["INFORMATION" on page 114](#), with a subject keyword such as one of the following as argument: STATE VARIABLES, INTENSIVE VARIABLES, EXTENSIVE VARIABLES, DERIVED VARIABLES, CONDITIONS (for condition settings), AXIS-VARIABLES (for stepping/mapping variable settings).

Common Thermodynamic Variables

The tables below list common thermodynamic variables. Most of these can be used to define equilibrium conditions in the POLY module unless otherwise indicated.

The variables are divided into the following tables:

- Intensive variables
- Energy-related extensive variables for whole system or for a phase
- Compositional extensive variables (overall amount of components in the whole system, or amount of a component in system or in a phase)
- Constitutional composition-related extensive variables (amount of a constituent/species on a sublattice site in a phase)
- Special quantities

How to Read the Tables

- The *Abbrev.* column shows the abbreviation that you use in the POLY module for referring to the variable. If the variable must be given any arguments, then these are given in parenthesis directly after the abbreviation. For most variables, this is also the abbreviation that you use to refer to the variable in other modules. However, some variables are referred to with a different abbreviation in the POST module. If this is the case, then this is noted at the bottom of the table.
- Variables that are specific to a species, in which case the species is specified as an argument (*sp* in the table below). If there are two or more sublattices in a given phase, then this argument is given as *constituent#sublattice*. This indicates a constituent on a specific sublattice or site in the phase (referred to by the # sign and a digit). For example, *y*(BCC,C#2) stands for the site fraction of the C species on the second sublattice site of the BCC_A2 solution phase.
- The *Unit* column show which unit that you can use to express the variable in the POLY module. This unit is always the SI unit. In other modules, state variables may be expressed in other units.
- The *Suffix* column shows the suffixes you can append to the variables. The R-suffix can be used with all compositional extensive state variables, but the suffix does not always change the value of the variable. This is indicated by putting the *R* in parenthesis.

These types of variables are listed in the following topics:

- ["Intensive Variables" below](#)
- ["Extensive Variables" on the next page](#)
- ["Special Quantities" on page 388](#)
- ["The u-Fraction Variable" on page 389](#)
- ["Suffixes" on page 390](#)

Intensive Variables

| V | Abbrev. | Unit | Descript. | Domain | Suffix |
|---|----------------|------|-------------|--------|--------|
| T | T ¹ | K | Temperature | System | |
| P | P | Pa | Pressure | System | |

| V | Abbrev. | Unit | Descript. | Domain | Suffix |
|-------|---------------------------|-------|--------------------|--------------------------------------|--------|
| μ | MU(comp) | J/mol | Chemical potential | Component | R |
| | MU(sp,ph) ² | | | Species relative to a solution phase | R |
| a | AC(comp) | N/A | Activity | Component | R |
| | AC(sp,ph) ² | | | Species relative to a solution phase | R |
| | LNAC (comp) ³ | | ln(Activity) | Component | R |
| | LNAC (sp,ph) ² | | | Species relative to a solution phase | R |

¹ When plotting in POST, besides T (Kelvin), you can also use T_C or T_F to plot temperature in °C or °F.

² Only for single-substitutional-lattice solution phases such as AQUEOUS solution and GASEOUS mixture phases and for interacting species on the substitutional sublattice of two-sublattice solution phases (such as the phases BCC_A2 and M6C phases).

³ In natural logarithm (lnAC=MU/RT)

Extensive Variables

ENERGY-RELATED EXTENSIVE VARIABLES FOR WHOLE SYSTEM OR FOR A PHASE

| V | Abbrev. | Unit | Descript. | Domain | Suffix |
|---|---------------------|----------------|------------------|--------|---------------|
| V | V | m ³ | Volume | System | M, W, V, R |
| | V(ph) ¹ | | | Phase | M, W, F, R |
| | VP(ph) ² | | | Phase | M, W, V, R |
| G | G | J | Gibbs energy | System | M, W, V, R |
| | G(ph) ¹ | | | Phase | M, W, V, F, R |
| A | A | J | Helmholtz energy | System | M, W, V, R |
| | A(ph) ¹ | | | Phase | M, W, V, F, R |

| V | Abbrev. | Unit | Descript. | Domain | Suffix |
|----|-----------------------|---------|--------------------------------------|--------|---------------------------------------------------|
| U | U | J | Internal energy | System | M, W, V, R |
| | U(ph) ¹ | | | Phase | M, W, V, F, R |
| H | H | J | Enthalpy ⁶ | System | M, W, V, R |
| | H(ph) | | | Phase | M, W, V, F |
| S | S | J/K | Entropy ⁶ | System | M, W, V, R |
| | S(ph) ¹ | | | Phase | M, W, V, F, R |
| Cp | HM.T ³ | J/mol/K | Heat capacity at constant pressure | System | R |
| | HM(ph).T ³ | | | Phase | R |
| Cv | HM.T ⁴ | J/mol/K | Heat capacity at constant volume | System | R |
| | HM(ph).T ⁴ | | | Phase | R |
| D | DG(ph) ⁵ | N/A | Driving force (thermodynamic factor) | Phase | Always use with M, W, V or F. R can also be used. |

¹ For this variable, if the phase is unstable, then the variable gets a value of zero.

² Do not use VP(ph) as a condition in POLY. Instead, use `CHANGE_STATUS PHASE <PHASE>=FIX <AMOUNT>` where the fixed <AMOUNT> is roughly equal to VPF(ph), which cannot be directly evaluated or listed. If the phase is unstable, then VP(ph) and its normalized quantities get zero value.

³ Use only if pressure has been set as a condition.

⁴ Use only if volume has been set as a condition.

⁵ Already divided by RT.

⁶ When working in the POST module you can also enter the abbreviation for this variable into the Console, for example, `enth` or `enthalpy`, which corresponds to HM, and `entr` and `entropy`, which corresponds to SM.

COMPOSITIONAL EXTENSIVE VARIABLES

These are for the overall amount of components in whole system, or amount of a component in system or in a phase.

Do not use NP(ph) or BP(ph) as conditions in the POLY module. Instead use `CHANGE_STATUS PHASE <PHASE>=FIX <AMOUNT>` where the fixed <AMOUNT> is roughly equal to NPF(ph) or BPF(ph), which cannot be directly evaluated or listed. If the phase is unstable, then NP(ph) or BP(ph) (and its normalized quantities) get zero value.

When plotting the following quantities in POST, refer to each as indicated:

- $X(\text{comp}) \rightarrow \text{Mole-Fraction } \langle \text{comp} \rangle$ (or M_F)
- $W(\text{comp}) \rightarrow \text{Weight-Fraction } \langle \text{comp} \rangle$ (or W_F)
- $X\%(\text{comp}) \rightarrow \text{Mole-Percent } \langle \text{comp} \rangle$ (or M_P)
- $W\%(\text{comp}) \rightarrow \text{Weight-Percent } \langle \text{comp} \rangle$ (or W_P).
- $u-f(\text{ph}, \text{comp}) \rightarrow U-F$

| V | Abbrev. | Unit | Descript. | Domain | Suffix | Comment |
|---|---------------------|------|---------------|-------------------------|-----------------|-----------|
| n | N | mole | Moles | All components | M, W, V, (R) | |
| | N(comp) | | | Component | M, W, V, (R) | |
| | N (ph,comp) | | | Component in a phase | M, W, V, (R) | |
| | NP(ph) ¹ | | | Phase | M, W, V, (R) | See above |
| b | B | gram | Mass | All components | M, W, V, (R) | |
| | B(comp) | | | Component | M, W, V, (R) | |
| | B(ph,comp) | | | Component in a phase | M, W, V, (R) | |
| | BP(ph) ¹ | | | Phase | M, W, V, (R) | See above |
| x | X(comp) | N/A | Mole fraction | Component | (R) | See above |
| | X(ph,comp) | | | Component in a phase | (R) | |

| V | Abbrev. | Unit | Descript. | Domain | Suffix | Comment |
|-----------------------------------------------------------------------------------------------------------------------|---------------------------|------|------------------------|-----------------------------|--------|-----------|
| w | W(comp) | N/A | Mass (weight) fraction | Component | (R) | See above |
| | W(ph,comp) | | | Component in a phase | (R) | |
| x% | X%(comp) ² | N/A | Mole percent | Component | (R) | See above |
| w% | W%(comp) ² | N/A | Mass (weight) percent | Component | (R) | See above |
| u | u-f(ph,comp) ¹ | N/A | u-fraction | Component in a stable phase | (R) | See above |
| in | IN(sp) ² | mole | Input mole number | Phase species in the system | (R) | See above |
| im | IM(sp) ² | gram | Input mass unit | Phase species in the system | (R) | See above |
| ¹ Do not use as a condition in the POLY module. ² Only available in TQ-Interface and TC-API. | | | | | | |

CONSTITUTIONAL COMPOSITION-RELATED EXTENSIVE VARIABLE

This is the amount of a constituent/species on a sublattice site in a phase.

| V | Abbrev. | Unit | Descript. | Domain |
|---|----------------|------|---------------|------------------------------------------------------------------------|
| y | Y(ph,cons#sub) | N/A | Site fraction | Constituent on a sublattice site (denoted by # and a digit) in a phase |

Special Quantities

| Variable | Abbrev. | Unit | Description or Example | Domain | Suffix |
|----------|---------------------|------|--------------------------|--------|----------------------------------------------------------------|
| Q | QF(ph) ¹ | n/a | Phase stability function | Phase | R Under a condition and system definition, QFR(ph) = QF(ph) |

| Variable | Abbrev. | Unit | Description or Example | Domain | Suffix |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------|------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------|--------------------------------------------------------------------|
| Tc | TC(ph) ² | K | Curie temperature | Phase | R Under a condition and system definition, TCR(ph) = TC(ph) |
| Mb | BMAG(ph) ³ | n/a | Bohr magneton number | Phase | R Under a condition and system definition, BMAGR(ph) = BMAG(ph) |
| D1G | D1G(phase, site-fraction) | n/a | For example, D1G(FCC_A1#1, Cr#1) for first derivative of G for first composition set of FCC_A1 phase with respect to Cr site fraction on first sublattice. ▶ Search for TQGMDY in the <i>TQ-Interface Guide</i> | Phase | n/a |
| D2G | D2G(phase, site-fraction, site-fracton) | n/a | For example, D2G(FCC_A1#2, Cr#1, Cr#1) for second derivative of G for second composition set of FCC_A1 phase with respect to Cr site fraction on first sublattice. ▶ Search for TQDGY in the <i>TQ-Interface Guide</i> | Phase | n/a |
| <p>¹ Negative when phase composition is inside a spinodal, otherwise positive. Can be used to find out if an equilibrium is within the miscibility gap for a solution phase. Cannot be used as a condition.</p> <p>² Calculated for phases with magnetic contributions in an equilibrium state. Cannot be used as a condition, but can be plotted in POST or evaluated in POLY using SHOW_VALUE.</p> <p>³ Calculated for phases with magnetic contributions in an equilibrium state.</p> <p>n/a = not applicable</p> | | | | | |

The u-Fraction Variable

The u-fraction is an important quantity in some single-point or stepping paraequilibrium calculations in the POLY module and in the DICTRA module. You can apply the variable in a paraequilibrium calculation to the substitutional matrix component, the substitutional alloying components or the interstitial component. The u-fraction is denoted as u_i for the i -th system component n of a whole system or of a specific phase in various equilibrium states (such as full-equilibria, partial-equilibria, para-equilibria, local-equilibria).

Generally, the u-fraction is defined as:

$$\frac{x_i}{\sum_{j \in S} x_j}$$

The sum of x_j in the denominator is calculated for all substitutional alloying elements in the whole system or in a specific phase. The variable x_i in the numerator stands for the mole-fraction of the i -th component in the whole system or in the specific phase.

Suffixes

Suffixes may be appended to all extensive variables and to some intensive variables. Some suffixes can be used to enter the value of variables in normalized form. These are referred to as normalizing suffixes. If the variable that you create with a normalizing suffix is based on a state variable that can be set as a condition in POLY, then the normalized variable can also be set as a condition in POLY.

The normalizing suffixes are M (per mole), W (per mass in gram), V (per volume in m³) and F (per mole formula unit). There is also a reference state suffix _R, which you can use if you want the value of a thermodynamic variable to be calculated with respect to a reference state that have previously set.

Normalizing Suffixes

When variables that express system and phase quantities are normalized, the following general rules are used:

- System quantities are normalized by the total system size (in terms of N, B or V).
- Phase quantities are normalized by the phase amount [in terms of NP(ph), BP(ph) or VP(ph)].

The normalized quantities of G(ph), A(ph), U(ph), H(ph), S(ph) and V(ph) are calculated according to the thermodynamic model used for the phase (e.g. GM(ph), AM(ph), UM(ph), HM(ph), SM(ph) and VM(ph)). These quantities are calculated using the first derivatives of the Gibbs energy expressed for the phase with respect to the current composition of the system.

The tables describe the normalizing suffixes for the different state variables.

G, A, U, H, S AND V OF A WHOLE SYSTEM

| Suffix | Description | Example |
|-----------------------------------|---------------------------------------------------------------------------|------------------------------------------------------------------------------------|
| M (per mole) | Total system size in terms of N. | GM is the Gibbs energy per mole of the system (J/mol). $GM = G/N$ |
| W (per mass in gram) | The total system size in terms of B. | GW is the Gibbs energy per mass of the system (J/g). $GW = G/B$ |
| V (per volume in m ³) | The total system size in terms of V. VV does not have to be evaluated. | GV is the Gibbs energy per volume of the system (J/m ³). $GV = G/V$ |

G(PH), A(PH), U(PH), H(PH), S(PH) AND V(PH) OF A PHASE

| Suffix | Example |
|-----------------------------------|---------------------------------------------------------------------------------------------------------------------------|
| M (per mole) | For example, GM(ph) is Gibbs energy of the phase per mole of the phase (J/mol). $GM(ph) = G(ph)/NP(ph)$ |
| W (per mass in gram) | For example, GW(ph) is Gibbs energy of the phase per mass of the phase (J/mol). $GW(ph) = G(ph)/BP(ph)$ |
| V (per volume in m ³) | For example, GV(ph) is Gibbs energy of the phase per volume of the phase (J/mol). $GV(ph) = G(ph)/V(ph)$ |
| F (per mole formula unit) | For example, GF(ph) is the Gibbs energy of the phase per formula unit of the phase (J/mol). $GF(ph) = G(ph)/NP(ph)*NA$ |

DG(PH) OF A PHASE

| Suffix | Description | Example(s) |
|--------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------|
| M (per mole) | Theoretically, the first derivative of the variable with regard to the phase amount in terms of NP(ph). Since DG(ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead. | DGM(ph) is driving force for precipitation of the phase per mole of components. $DGM(ph) = \partial DG(ph)/\partial NP(ph)$ |

| Suffix | Description | Example(s) |
|-----------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | DGM(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state. | |
| W (per mass in gram) | <p>Theoretically, the first derivative of the variable with regard to the phase amount in terms of BP(ph). Since DG(ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead.</p> <p>DGW(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.</p> | <p>DGW(ph) is driving force for precipitation of the phase per mass of components.</p> <p>$DGW(ph) = \partial DG(ph) / \partial BP(ph)$</p> |
| V (per volume in m ³) | <p>Theoretically, the first derivative of the variable with regard to the phase amount in terms of VP(ph). Since DG(ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead.</p> <p>DGV(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.</p> | <p>DGV(ph) is driving force for precipitation of the phase per volume of components.</p> <p>$DGV(ph) = \partial DG(ph) / \partial VP(ph)$</p> |
| F (per mole formula unit) | <p>Theoretically, the first derivative of the variable with regard to the phase amount in terms of NP(ph) and NA (NA is the total atomic number in the phase formula). Since DG(ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead.</p> <p>DGF(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.</p> | <p>DGF(ph) is driving force for precipitation of the phase per formula unit of components.</p> <p>$DGF(ph) = \partial DG(ph) / \partial NP(ph) \cdot \partial NA$</p> |

N AND B OF A SYSTEM

| Suffix | Description | Example(s) |
|----------------------|------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------|
| M (per mole) | <p>The total system size in terms of N.</p> <p>NM does not have to be evaluated.</p> <p>BM cannot be set as a condition.</p> | <p>BM is mass (gram) of components per mole of the system (g/mol).</p> <p>$BM = B/N$</p> |
| W (per mass in gram) | The total system size in terms of B. | NW is mole number of components per mass of the system (mol/g). |

| Suffix | Description | Example(s) |
|-----------------------------------|---------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | BW does not have to be evaluated. NW cannot be set as a condition. | $NW = N/B$ |
| V (per volume in m ³) | The total system size in terms of V. BV is the density of the entire system. | NV is mole number of components per volume of the system (mol/m ³). $NV = N/V$ BV is the density of the entire system (g/m ³). $BV = B/V$ |

N (COMP) AND B(COMP) OF A COMPONENT IN THE SYSTEM

| Suffix | Description | Example(s) |
|-----------------------------------|--------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------|
| M (per mole) | The total system size in terms of N. BM(comp) cannot be set as a condition. | NM(comp) is the mole of a component per mole of the system (i.e. mole fraction, which also is expressed as X(comp)). $NM(comp) = N(comp)/N$ |
| W (per mass in gram) | The total system size in terms of B. NW(comp) cannot be set as a condition. | BW(comp) is mass (gram) of a component per mass of the system (i.e. mass fraction, which also is expressed as W(comp)). $BW(comp) = B(comp)/B$ |
| V (per volume in m ³) | The total system size in terms of V. | NV(comp) is mole number of a component per volume of the system (mol/m ³). $NV(comp) = N(comp)/V$ |

NP(PH), BP(PH) AND VP(PH) OF A PHASE IN THE SYSTEM

| Suffix | Description | Example(s) |
|--------------|------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| M (per mole) | BPM(ph) and VPM(ph): The phase amount in terms of NP(ph). NPM(ph): The total system size in terms of N. | BPM(ph) is mass (gram) of a phase per moles of the system (g/mol). $BPM(ph) = BP(ph)/N$ NPM(ph) is number of moles of a phase per moles of the system (mole fraction). $NPM(ph) = NP(ph)/N$ |

| Suffix | Description | Example(s) |
|-----------------------------------|------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| W (per mass in gram) | NPW(ph) and VPW(ph): The phase amount in terms of BP(ph). BPW(ph):The total system size in terms of B. | VPW(ph) is volume (m ³) of a phase per mass of the system (m ³ /g) $VPW(ph) = VP(ph)/B$ BPW(ph) is mass (gram) of a phase per mass of the system (mass fraction) $BPW(ph) = BP(ph)/B$ |
| V (per volume in m ³) | NPV(ph) and BPV(ph): The phase amount in terms of VP(ph). VPV(ph): The total system size in terms of V. | NPV(ph) is number of moles of a phase per volume of the system (mol/m ³). $NPV(ph) = NP(ph)/V$ VPV(ph) is volume (m ³) of a phase per volume of the system (volume fraction). $VPV(ph) = VP(ph)/V$ |

N(ph,comp) AND B(ph,comp) OF A COMPONENT IN A PHASE

| Suffix | Description | Example(s) |
|-----------------------------------|---------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| M (per mole) | The phase amount in terms of NP(ph) of the phase. | NM(ph,comp) is number of moles of a component per mole of a phase (i.e. mole fraction of a component in a phase, which is equivalent to X (ph, comp)). $NM(ph,comp) = N(ph,comp)/NP(ph)$ |
| W (per mass in gram) | The phase amount in terms of BP(ph) of the phase. | BW(ph,comp) is mass (gram) of a component per mass of a phase (i.e. mass fraction of a component in a phase, which is equivalent to W (ph,comp)). $BW(ph,comp) = B(ph,comp)/BP(ph)$ |
| V (per volume in m ³) | The phase amount in terms of VP(ph) of the phase. | NV(ph,comp) is mole number of a component per volume of a phase (mol/m ³). $NV(ph,comp) = N(ph,comp)/VP(ph)$ |

THE REFERENCE STATE SUFFIX R

You can use the reference state suffix _R for some thermodynamic variables to calculate their value with respect to a reference state that you have previously set for a system component with the ["SET_REFERENCE_STATE" on page 185](#) command in POLY (or in a response-driven

modules such as the POURBAIX module). The value of energy-related variables that are used with the \mathcal{R} suffix depends on the reference states of all the components in the defined system.



It is possible to use an \mathcal{R} suffix on all compositional extensive state variables as well, but the value of the state variable is always the same, with or without the suffix.

If the reference state for a system component is the default reference state (the stable reference state (SER) which is defined in a Thermo-Calc database), then $MUR(comp) = MU(comp)$, $ACR(comp) = AC(comp)$ and $LNACR(comp) = LNAC(comp)$.

In the case of some thermodynamic variables, you can also use the \mathcal{R} suffix to express chemical potentials and activities of species relative to some single-substitutional-lattice solution phases (such as aqueous solution, gaseous mixture, metallic liquid solution, slag mixture or MO solid solution). These state variables are $MU(sp,ph)$, $MUR(sp,ph)$, $AC(sp,ph)$, $ACR(sp,ph)$, $LNAC(sp,ph)$ and $LNACR(sp,ph)$.

The reference states and standard states of various solution species are pre-defined for some solution phases in some databases. For all solution species in any solution model in any database, it is always the case that $MUR(sp,ph) = MU(sp,ph)$, $ACR(sp,ph) = AC(sp,ph)$ and $LNACR(sp,ph) = LNAC(sp,ph)$.

Derived Variables and Partial Derivatives

Many derived variables can be obtained easily by using partial derivatives of state variables, such as heat capacity, thermal expansivity, isothermal compressibility, among others.

Derivatives of state variables can be defined or evaluated by putting a dot (.) between two state variables. The variable after the dot must be a condition that you have set when you defined your system. For example, the heat capacity (at constant pressure or volume) of a system is the partial derivative of the state variable enthalpy with respect to temperature. To evaluate this derivative, use the designation $HM.T$, where temperature is a state variable that you have set already.

Any partial derivative of a state variable with respect to another can be defined or evaluated as a derived variable by using the dot (.) notation.

DERIVED VARIABLES DOT NOTATION EXAMPLES

The following table shows some examples:

| Derived variable | Description |
|----------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| H | Heat capacity for the system at either constant P if pressure is a condition or constant V if volume is a condition. |
| H_M | Heat capacity for a phase at either constant P if pressure is a condition or constant V if volume is a condition. |
| H | Heat capacity for the system multiplied by total mole number of components, i.e., $\partial H/\partial T = C_p \cdot N$ if pressure is a condition in a closed system or $\partial H/\partial T = C_v \cdot N$ if volume is a condition in a closed system. |
| $H(ph), T = \partial H(ph)/\partial T$ | Heat capacity for a phase multiplied by the sum of $NP(ph)$ and $HM(ph) \cdot \partial NP(ph)/\partial T$, i.e., $C_p(ph) \cdot NP(ph) + HM(ph) \cdot \partial NP(ph)/\partial T$ if pressure is a condition or $C_v(ph) \cdot NP(ph) + HM(ph) \cdot \partial NP(ph)/\partial T$ if volume is a condition. |
| $VM, T = \partial VM/\partial T$ | Thermal expansivity of the system (already multiplied by the total molar volume), i.e., $\partial VM/\partial T = \alpha \cdot VM$. |
| $VM(ph), T = \partial VM(ph)/\partial T$ | Thermal expansivity of a phase (already multiplied by its molar volume), i.e., $\partial VM(ph)/\partial T = \alpha(ph) \cdot VM(ph)$. |
| $V, T = \partial V/\partial T$ | Thermal expansivity of the system (already multiplied by the total volume), i.e., $\partial V/\partial T = \alpha \cdot V$. |
| $V(ph), T = \partial V(ph)/\partial T$ | Thermal expansivity of a phase (already multiplied by the phase volume) plus the $VM(ph) \cdot \partial NP(ph)/\partial T$ term, i.e., $\partial V(ph)/\partial T = \alpha(ph) \cdot V(ph) = \alpha(ph) \cdot VM(ph) \cdot NP(ph) + VM(ph) \cdot \partial NP(ph)/\partial T$. |
| $VM, P = -\partial VM/\partial P$ | Isothermal compressibility of the system (already multiplied by the total molar volume), i.e., $\partial VM/\partial P = -\kappa \cdot VM$. |
| $VM(ph), P = -\partial VM(ph)/\partial P$ | Isothermal compressibility of a phase (already multiplied by its molar volume), i.e., $\partial VM(ph)/\partial P = -\kappa(ph) \cdot VM(ph)$. |
| $V, P = -\partial V/\partial P$ | Isothermal compressibility of the system (already multiplied by the total volume), i.e., $\partial V/\partial P = -\kappa \cdot V$. |
| $V(ph), P = -\partial V(ph)/\partial P$ | Isothermal compressibility of a phase (already multiplied by the phase volume) plus the $VM(ph) \cdot \partial NP(ph)/\partial P$ term, i.e., $\partial V(ph)/\partial P = -\kappa(ph) \cdot V(ph) = -\kappa(ph) \cdot VM(ph) \cdot NP(ph) + VM(ph) \cdot \partial NP(ph)/\partial P$. |
| $T, X(comp) = \partial T/\partial X(comp)$ | Slope of a phase boundary on a T-X(comp) phase diagram with respect to mole fraction of the component in the system. |
| $T, W(comp) = \partial T/\partial W(comp)$ | Slope of a phase boundary on a T-W(comp) phase diagram with respect to mass of the component in the system. |
| $T, X(ph, comp) = \partial T/\partial X(ph, comp)$ | Slope of a phase boundary on a T-X(ph, comp) phase diagram with respect to mole fraction of the component in the phase. |

| Derived variable | Description |
|-------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------|
| $\frac{\partial W(\text{ph,comp})}{\partial T} = \frac{\partial W(\text{ph,comp})}{\partial T}$ | Slope of a phase boundary on a T-W(ph,comp) phase diagram with respect to mole fraction of the component in the phase. |
| $P.T = \partial P / \partial T$ | Slope of a phase boundary on a P-T phase diagram (Note that the equilibrium with phase assemblage must be calculated first). |

Defining New Derived Variables and Functions

You can define additional derived variables or functions based on a state variable by using ENTER_SYMBOL. Any derived variable or function must have a unique name that starts with a letter and has a maximum number of eight characters. These characters can include both uppercase and lowercase letters, numerical digits and the underscore (_). No other characters are allowed.

The difference between new derived variables introduced with the ENTER_SYMBOL command and new functions introduced with the same command is as follows. Whenever Thermo-Calc calculates the value of a function (as part of an equilibrium calculation for example), all functions related to the defined system is evaluated. An entered derived variable, on the other hand, is only evaluated when it is defined and when it is re-evaluated with EVALUATE_FUNCTIONS.

Derived Variables for Aqueous Solutions

Standard state variables used for other phases can be directly applied to the aqueous solution phase. In addition, there are pre-defined derived variables for the aqueous solution phase in particular.

Examples of predefined derived variables for the aqueous solution phase are listed and briefly described in the following tables. Some derived variables for a gaseous mixture phase are also shown. This is because EOS (Equation of State) expressions, standard thermodynamic properties and transport properties of the pure solvent H2O are also expressions and properties of the pure gaseous species H2O.

FOR AQUEOUS SOLUTION PHASE

| Name | Abbrev. | Units | Description | Comments |
|------|---------|-------|---------------------------------|----------------------------------------------------------------------------------------------------------------------------------|
| pH | PH | N/A | Acidity | of the aqueous solution phase $\text{pH} = -\log_{10}(\text{AC}(\text{H}^+)) = -\log_{10}(\text{ACR}(\text{H}^+, \text{AQ}))$ |
| Eh | EH | V, mV | Hypothetical electric potential | of the aqueous solution phase $\text{Eh} = u(\text{ZE})/96485.309$ |

| Name | Abbrev. | Units | Description | Comments |
|------------|---------|---------------------|-------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------|
| Pe | PE | N/A | Logarithm of the hypothetical electron activity | of the aqueous solution phase $pe = u(ZE)/(2.3025851 \cdot RT)$ |
| Ah | AH | kJ, kcal | Thermodynamic affinity per electron | of a redox couple wrt the standard hydrogen electrode in the aqueous solution phase $Ah = u(ZE)$ |
| yw | YH2O | N/A | Mole fraction | of the solvent H2O in the aqueous solution phase $YH2O = Y(AQ, H2O)$ |
| Nw | AH2O | mole | Mole number | of 1.0 kg of solvent H2O $AH2O = 55.508435$ |
| Nsp | NSH2O | mole | Mole number, $NS(AQ, H2O)$ | of the solvent (H2O) in the aqueous solution phase $NS(AQ, H2O) = YH2O \cdot NP(AQ)$ |
| | NS# | | Mole number, $NS(AQ, sp)$ | of a solute species in the aqueous solution phase $NS(AQ, sp) = Y(AQ, sp) \cdot NP(AQ)$ |
| M | ML# | mol/kg_H2O | Molality, $ML(AQ, sp)$ | of a solute species in the aqueous phase $ML(AQ, sp) = Y(AQ, sp) \cdot AH2O / YH2O$ |
| m* | TIM | equivalent molality | Total molality | of all solute species in the aqueous solution phase $TIM = \sum [ML(AQ, sp)]_{ions} + \sum [ML(AQ, sp)]_{complexes}$ |
| mt | TIC# | equivalent molality | Total ionic concentration, $TIC(AQ, sp)$ | of a cation I in the aqueous phase $TIC(AQ, spI) = \sum [ML(AQ, spI)] \cdot V(spI-in-spI)]$ |
| I | ISTR | N/A | Ionic strength | of the aqueous solution phase $ISTR = 1/2 \cdot \sum [ML(AQ, sp) \cdot Z(AQ, sp)^2]$ |
| γ | RCH2O | N/A | Activity coefficient, $RC(H2O, AQ)$ | of the solvent (H2O) $RC(H2O, AQ) = ACR(H2O, AQ) / YH2O$ |
| | RC# | | Activity coefficient, $RC(sp, AQ)$ | of a solute species $RC(sp, AQ) = ACR(sp, AQ) / Y(AQ, sp) \cdot YH2O$ |
| α_i | AIH2O | N/A | Activity, $AI(H2O, AQ)$ | of the solvent (H2O), $AI(H2O, AQ) = ACR(H2O, AQ)$ |
| | AI# | | Activity, | of a solute species related to the aqueous solution phase, |

| Name | Abbrev. | Units | Description | Comments |
|------------|---------|--------------------------|---------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | | | Al(sp,AQ) | Al(sp,AQ) = ACR(sp,AQ)*AH2O |
| | LogAl# | | Log10 Activity, LogAl(H2O,AQ), LogAl(sp,AQ) | of the solvent or a solute species related to the aqueous solution phase in common logarithm, LogAl(H2O,AQ) = log10[Al(H2O,AQ)] LogAl(sp,AQ) = log10[Al(sp,AQ)] |
| α_w | AW | N/A | Activity | of H2O in the aqueous solution phase AW = ACR(H2O,AQ) |
| ϕ | OS | N/A | Osmotic coefficient | of aqueous solution phase OS = -55.508435*lnAW/TIM |
| At1 | AT1 | equil_ mol/kg_ H2O | Titration alkalinity (definition 1) | of the aqueous solution phase Generally defined as the equivalent molality of carbonate and bicarbonate at the methyl orange endpoint (pH=4.5). |
| At2 | AT2 | equil_ mol/kg_ H2O | Titration alkalinity (definition 2) | of the aqueous solution phase Generally defined as the equivalent molality of carbonate and bicarbonate, plus sulfide, at the methyl orange endpoint (pH=4.5). |

FOR GASEOUS MIXTURE PHASE

| Name | Abbrev. | Units | Description | Comments |
|------------|---------|--------------|-------------------------------------|------------------------------------------------------------------------------------------------|
| γ | RA# | N/A | Activity coefficient, RA(sp,GAS) | of a gaseous species in the gaseous mixture RA(sp,GAS) = function(Y,T,P) |
| γ^* | RF# | N/A | Fugacity coefficient, RF(sp,GAS) | of a pure gaseous species under TP RF(sp,GAS) = function(T,P/V) |
| F | FUG# | pa, bar, psi | Fugacity, FUG(sp,GAS) | of a gaseous species in the gaseous mixture FUG(sp,GAS) = RA(sp,GAS)*RF(sp,GAS)*Y(GAS,sp)*P |
| ft | TFUG | pa, bar, psi | Total gas fugacity | of the gaseous mixture phase TFUG = sum[FUG(sp,GAS)] |

Defining New Derived Variables for Aqueous Solutions

You can define many different additional derived variables and functions. For instance, the partition coefficient of a component between two phases is defined as follows:

$$Pc<name> = X(phase1, component) / X(phase2, component)$$

Another example is the activity coefficient of a component in the system. It is defined as follows:

$$Rc<name> = ACR(component) / X(component)$$

The activity coefficient of a species in a solution phase depends on which model definitions on the reference states that are used and it depends on the standard states for the species. If the standard state of a species is defined to be the same as the pure species in a substitutional phase, then the activity coefficient of the species can be calculated as:

$$RC<name> = ACR(species, phase) / Y(phase, species)$$

In some cases, there are more than one sublattice in the phase and the reference states for the phase species cannot be presented by the pure species, as in the case of C in FCC [(Fe)1 (C,N,VA)1], where the model may end at fifty percent C and fifty percent Fe. In those cases, the chemical potential and activity of all phase constituents is not well defined and you cannot properly define the activity coefficients of the species in the phase.

For an aqueous solution phase, no matter what model is used, the reference state and standard state for both the solvent and solutes are defined in a special way in the Thermo-Calc software. The reference state for the solvent is set as pure water, the same as its standard state (according to Raoult's Law). The standard state for a solute species is set the hypothetical solute species, whilst its reference state is defined as the hypothetical state at unit molality (one mole dissolved into 1.0 kg of solvent) but in which the environment of each molecular is the same as at infinite dilution (according to Henry's Law). Under these definitions, the activity coefficients for solvent species can be calculated as follows:

$$RC<H2O> = ACR(H2O, aqueous) / Y(aqueous, H2O)$$

The coefficients for the solute species can be calculated as follows:

$$\begin{aligned} RC<spec> &= AI(species, aqueous) / ML(aqueous, species) \\ &= ACR(species, aqueous) / Y(aqueous, species) * Y(aqueous, H2O) \end{aligned}$$

AI is here the activity of solute species calculated from the model, and ML is the molality of the species.

Thermodynamic Variables and Wildcard Characters

The ACR (species, phase) and the MUR (species, phase) quantities can only be appropriately and meaningfully applied to substitutional solution phases (such as GAS, AQUEOUS, LIQUID) and to solution phases without an interstitial sublattice set. This means that the wild card characters * and \$ normally don't work properly for the activity and/or chemical potential properties.

For example, do not use `ACR(*,*)` or `MUR(*,*)` for all the species relative to all phases, nor `ACR(*,phase)` or `MUR(*,phase)` for all the species relative to a specific phase, nor `ACR(species,*)` or `MUR(species,*)` for a specific species relative to all phases.

Instead, use specific names for species and (applicable) phase, as in the following examples:

```
SHOW_VALUE acr(fe+2,aqueous)Lists activity of the Fe+2 species in AQUEOUS solution  
phase
```

```
SHOW_VALUE mur(c2,gas)Lists chemical potential of the C2 species in GAS mixture  
phase
```

```
SET_AXIS_VAR y ac(o2,gas)Sets activity of the O2 species in GAS mixture phase as Y-  
axis
```

Units of State Variables and Derived Variables

The units for the state variables in the Units column in the table in ["User-Specified Units" below](#) are the SI units that are used in the POLY module. However, in the POST module, you can both use pre-defined symbols and define your own symbols which are based on state variables and derived variables. By doing this, you can express the value of the thermodynamic variables in non-default units. The following topic briefly describes how you can create your own symbols and suggests expressions that you can use to convert default units into other standard units which are not default units in Thermo-Calc.

The topic ["Examples of User-Defined Units" below](#) describes some variables of specific species in a phase and the units in which they are expressed. These variables are not used in POLY or POST, but in the GIBBS, DATA, PARROT and ED_EXP modules.

User-Specified Units

You do not always need to use the default units for variables. Using ["ENTER_SYMBOL" on page 167](#), you can convert the value of variable from the default unit to your preferred unit. (Some response-driven modules also allow you to set conditions in non-default units.) User-defined symbols in the form of functions can be used for plotting in the POST module, but they cannot be used as conditions in POLY. User defined symbols in the form of variables can be used as conditions.

For example, if you want pressure to be plotted in bar rather than Pa, then you define the following function PB:

```
Enter_symbol function PB = P/1E5 ;
```

If you wanted heat capacity of a system to be shown as in terms of J/mol/K, then you can define the following function Cp:

```
Enter_symbol function Cp = Hm.T ;
```

If the variable you want to convert is a function of one or more derivatives, then you must enter the symbol as a variable rather as a function. For instance, a symbol expressing heat capacity of a system in a unit of cal/mol/K can be defined as the following variable Cp2:

```
Enter_symbol variable Cp2 = Hm.T/4.1858 ;
```



Also see ["Examples of User-Defined Units" below](#) for information about entering conventional functions and the associated units.

Examples of User-Defined Units

The following tables give examples of expressions you can use to enter symbols. This enables you to show the values of thermodynamic variables in a variety of units.

▶ ["Units of State Variables and Derived Variables" on the previous page](#) and ["User-Specified Units" on the previous page](#)



You can also use thermodynamic variables with normalizing suffixes in the expression when you enter a symbol. However, the tables do not have examples of these expressions.

In the expressions these are defined as follows:

- i is for an auxiliary index or letter that corresponds to the component c
- j is for an auxiliary index or letter that corresponds to the phase ph , and
- ij stands for an auxiliary index or letter that corresponds to the component c in the phase ph .

INTENSIVE AND EXTENSIVE VARIABLES OF A DEFINED SYSTEM

| Quantity | Suggested name and expression | Unit |
|----------------------------------------------------|-----------------------------------|--------------------------|
| <i>For intensive variables of a defined system</i> | | |
| Temperature | TempC = $T - 273.15$ | Celsius (C) |
| | TempF = $1.8 * T - 459.67$ | Fahrenheit (F) |
| | TempF = $1.8 * \text{TempC} + 32$ | |
| Pressure | PB = $P / 1E5$ | bars (bar) |
| | PKb = $P / 1E8$ | kilobars (kbar) |
| | PAtm = $P / 101325$ | atmosphere (atm) |
| | PSI = $P / 6894.76$ | pounds/sq. inch (psi) |
| | PIHg = $P / 3342.11$ | inches of Hg |
| | PTor = $P / 133.322$ | Tors (millimeters of Hg) |
| <i>For extensive variables of a defined system</i> | | |
| Amount | BKg = $1E-3 * B$ | kilograms (kg) |
| | BTon = $1E-6 * B$ | tons |

| Quantity | Suggested name and expression | Unit |
|----------------------------|----------------------------------|----------------------------------------|
| Volume | $VDM = 1E-3 \cdot V$ | cubic decimeters (dm ³ , l) |
| | $VCM = 1E-6 \cdot V$ | cubic centimeters (cm ³) |
| | $VMM = 1E-9 \cdot V$ | cubic millimeters (mm ³) |
| | $VCI = 1.6387064E-5 \cdot V$ | cubic inches (in ³) |
| | $VLi = 1E-3 \cdot V$ | liters (l) |
| Energy | $GCal = G/4.1858$ | cal |
| | $ACal = A/4.1858$ | cal |
| | $UCal = U/4.1858$ | cal |
| | $HCal = H/4.1858$ | cal |
| | $SCal = S/4.1858$ | Cal/K |
| Heat Capacity | $Cp2 = HM.T/4.1858$ | cal/mol/K |
| | $Cp3 = HW.T/4.1858$ | cal/g/K |
| | $Cp4 = HV.T/4.1858$ | cal/m ³ /K |
| Thermal Expansion | $A2 = VM.T \cdot 1E-6 \cdot VM$ | cm ³ /mol/K |
| | $A3 = VW.T \cdot 1E-6 \cdot VM$ | cm ³ /g/K |
| Isothermal Compressibility | $B2 = -VM.P \cdot 1E-9 \cdot VM$ | mm ³ /mol/Pa |
| | $B3 = -VW.P \cdot 1E-9 \cdot VM$ | mm ³ /g/Pa |

INTENSIVE AND EXTENSIVE VARIABLES OF A SYSTEM COMPONENT

| Quantity | Suggested name and expression | Unit |
|------------------------------------------------------|------------------------------------------|---------------|
| <i>For intensive variables of a system component</i> | | |
| Chemical Potential | $MU_i = MU(c)/4.1858$ | cal/mol |
| | $MUR_i = MUR(c)/4.1858$ | cal/mol |
| Special quantity for aqueous solution | $pH = -\text{LOG}_{10}(ACR(H+1))$ | dimensionless |
| | $Eh = MUR(ZE)/RNF$ where $RNF=96485.309$ | volts (V) |

| Quantity | Suggested name and expression | Unit |
|------------------------------------------------------|-------------------------------|----------------|
| <i>For extensive variables of a system component</i> | | |
| Amount | $MF_i = N(c)/N = X(c)$ | dimensionless |
| | $MP_i = N(c)/N \cdot 100$ | dimensionless |
| | $WF_i = B(c)/B = W(c)$ | dimensionless |
| | $WP_i = B(c)/B \cdot 100$ | dimensionless |
| | $BK_{gi} = 1E-3 \cdot B(c)$ | kilograms (kg) |
| | $BT_{oni} = 1E-6 \cdot B(c)$ | tons |

EXTENSIVE VARIABLES OF A PHASE

| Quantity | Suggested name and expression | Unit |
|----------|--------------------------------|----------------------------------------|
| Amount | $MF_j = NP(ph)/N$ | dimensionless |
| | $MP_j = NP(ph)/N \cdot 100$ | dimensionless |
| | $WF_j = BP(ph)/B$ | dimensionless |
| | $WP_j = BP(ph)/B \cdot 100$ | dimensionless |
| | $BK_{gj} = 1E-3 \cdot BP(ph)$ | kilograms (kg) |
| | $BT_{onj} = 1E-6 \cdot BP(ph)$ | tons |
| Volume | $VCM_j = 1E-3 \cdot V(ph)$ | cubic decimeters (dm ³ , l) |
| | $VCM_j = 1E-6 \cdot V(ph)$ | cubic centimeters (cm ³) |
| | $VMM_j = 1E-9 \cdot V(ph)$ | cubic millimeters (mm ³) |
| Energy | $GCal_j = G(ph)/4.1858$ | cal |
| | $ACal_j = A(ph)/4.1858$ | cal |
| | $UCal_j = U(ph)/4.1858$ | cal |
| | $HCal_j = H(ph)/4.1858$ | cal |
| | $SCal_j = S(ph)/4.1858$ | Cal/K |

| Quantity | Suggested name and expression | Unit |
|----------------------------|-------------------------------|-------------------------|
| Driving Force | $DG2j = DGM(ph)/4.1858$ | cal/mol |
| | $DG3j = DGW(ph)/4.1858$ | cal/g |
| | $DG4j = DGV(ph)/4.1858$ | Cal/m ³ |
| | $DG5j = DGF(ph)/4.1858$ | cal/mole_formula_unit |
| Heat Capacity | $Cp2j = HM(ph).T/4.1858$ | cal/mol/K |
| | $Cp3j = HW(ph).T/4.1858$ | cal/g/K |
| | $Cp4j = HV(ph)/.T/4.1858$ | cal/m ³ /K |
| | $Cp5j = HF(ph)/.T/4.1858$ | cal/mole_formula_unit/K |
| Thermal Expansion | $A2j = VM(ph).T/VM(ph)$ | 1/K |
| Isothermal Compressibility | $B2j = -VM(ph).P/VM(ph)$ | 1/Pa |

EXTENSIVE VARIABLES OF A COMPONENT IN A PHASE

| Quantity | Suggested name and expression | Unit |
|----------|-----------------------------------|----------------|
| Amount | $MFij = N(ph,c)/NP(ph) = X(ph,c)$ | dimensionless |
| | $MPij = N(ph,c)/NP(ph)*100$ | dimensionless |
| | $WFi = B(ph,c)/BP(ph) = W(ph,c)$ | dimensionless |
| | $WPij = B(ph,c)/BP(ph)*100$ | dimensionless |
| | $BKgij = 1E-3*B(ph,c)$ | kilograms (kg) |
| | $BTonij = 1E-6*B(ph,c)$ | tons |

INTENSIVE AND EXTENSIVE VARIABLES OF A SPECIES IN A PHASE

| Quantity | Suggested name and expression | Unit |
|--------------------------------------------------------|-------------------------------|---------|
| <i>For intensive variables of a species in a phase</i> | | |
| Chemical Potential | $MUCalij = MU(sp,ph)/4.1858$ | cal/mol |
| | $MUErgij = MU(sp,ph)*1E7$ | cal/mol |

| Quantity | Suggested name and expression | Unit |
|---------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------|
| Fugacity | $FA_{ij} = AC(sp,ph)*PATM$ | atmosphere (atm) |
| | $FB_{ij} = AC(sp,ph)*PB$ | bars (bar) |
| | $FC_{ij} = AC(sp,ph)*PKB$ | kilobars (kbar) |
| | $FT_{ij} = AC(sp,ph)*PTOR$ | Tors (millimeters of Hg) |
| ln(Fugacity) | $LnFA_{ij} = LNAC(sp,ph)+LN(PATM)$ | atmosphere (atm) |
| | $LnFB_{ij} = LNAC(sp,ph)+LN(PB)$ | bars (bar) |
| | $LnFC_{ij} = LNAC(sp,ph)+LN(PKB)$ | kilobars (kbar) |
| | $LnFT_{ij} = LNAC(sp,ph)+LN(PTOR)$ | Tors (millimeters of Hg) |
| Special quantity for aqueous solution | $Al_{ij}=ACR(Fe+3,AQ)*AH2O$ | dimensionless |
| | $RC_{ij}=ACR(Fe+3,AQ)*YH2O/Y(AQ,Fe+3)$ where $AH2O=55.508435$ and $YH2O=Y(AQ,H2O)$ | dimensionless |
| | $WRC_{lij} = WR(AQ,sp)/4.1858$ ($WR(AQ,sp)$ is only valid for aqueous species in a system in which the AQUEOUS solution phase is considered) | cal/mol |
| | <i>For extensive variables of a species in a phase</i> | |
| Special quantity for aqueous solution | $ML_{ij}=Y(AQ,Fe+3)*AH2O/YH2O$ | molality (m) |
| | $ISTR=1*IS1+1*IS2+1*IS3$ where $AH2O=55.508435$, $YH2O=Y(AQ,H2O)$ and $ISn=.5*MLi*Zi^{**2}+.5*MLj*Zj^{**2}+.5*MLk*Zk^{**2}$ | molality (m) |

UNITS FOR VARIABLES OF SPECIFIC SPECIES IN A PHASE

In the GIBBS, DATA, PARROT and ED_EXP modules, there are quantities that describe various thermodynamic, physical, chemical and transport properties for a compound phase, and for a certain species or a given species combination in a specific solution phase. The following table describes the units for those variables.



These variables cannot be directly used in the POLY or POST modules.

| Variables | Description and unit |
|----------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------|
| G(ph,sp) G(ph,sp;0) G(ph,sp1;sp2;...;0) | Gibbs energy (J/mol) of a pure substance or end-member. |
| G(ph,sp1,sp2,...) L(ph,sp1,sp2,...) G(ph,sp1,sp2,...;0) L(ph,sp1,sp2,...;0) G (ph,sp1,sp2,...;...;0) L (ph,sp1,sp2,...;...;0) | Zero-order interaction parameter (J/mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase. |
| G(ph,sp1,sp2,...;i) L(ph,sp1,sp2,...;i) G (ph,sp1,sp2,...;...;i) L (ph,sp1,sp2,...;...;i) | The ith -order interaction parameter (J/mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase. |
| TC(ph,sp) TC(ph,sp;0) TC (ph,sp1;sp2;...;0) | Curie temperature (K) of a pure substance or end-member. |
| TC(ph,sp1,sp2,...) TC(ph,sp1,sp2,...;0) TC (ph,sp1,sp2,...;...;0) | Zero-order Curie-temperature contribution (K) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase. |
| TC(ph,sp1,sp2,...;i) TC (ph,sp1,sp2,...;...;i) | The ith -order Curie-temperature contribution (K) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase. |
| BMAGN(ph,sp) BMAGN(ph,sp;0) BMAGN (ph,sp1;sp2;...;0) | Bohr magneton number (dimensionless) of a pure substance or end-member. |

| Variables | Description and unit |
|--------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| BMAGN (ph,sp1,sp2,...) | Zero-order Bohr magneton number (dimensionless) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase. |
| BMAGN (ph,sp1,sp2,...;0) | |
| BMAGN (ph,...;sp1,sp2,...;0) | |
| BMAGN (ph,sp1,sp2,...;i) | The ith -order Bohr magneton number (dimensionless) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase. |
| BMAGN (ph,sp1,sp2,...;...;i) | |
| V0(ph,sp) V0(ph,sp;0) V0 (ph,sp1;sp2,...;0) | Molar volume (m ³) at 1 bar and reference T0 of a pure substance or end-member. |
| V0(ph,sp1,sp2,...) V0 (ph,sp1,sp2,...;0) V0 (ph,sp1,sp2,...;...;0) | Zero-order composition-dependent molar volume (m ³) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase. |
| V0(ph,sp1,sp2,...;i) V0 (ph,sp1,sp2,...;...;i) | The ith-order composition-dependent molar volume (m ³) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase. |
| VA(ph,sp) VA(ph,sp;0) VA (ph,sp1;sp2,...;0) | Integrated thermal expansivity (m ³ /mol/K) of a pure substance or end-member. |
| VA(ph,sp1,sp2,...) VA (ph,sp1,sp2,...;0) VA (ph,sp1,sp2,...;...;0) | Zero-order composition-dependent thermal expansivity (m ³ /mol/K) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase. |
| VA(ph,sp1,sp2,...;i) VA (ph,sp1,sp2,...;...;i) | The ith -order composition-dependent thermal expansivity (m ³ /mol/K) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase. |
| VC(ph,sp) | High pressure fitting parameter (m ³ /mol) of a pure substance or endmember. |

| Variables | Description and unit |
|--------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| VC(ph,sp1,sp2,...) | Zero-order composition-dependent high pressure fitting parameter (m^3/mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase. |
| VC(ph,sp1,sp2,...i) | The ith -order composition-dependent high pressure fitting parameter (m^3/mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase. |
| VK(ph,sp) | Isothermal compressibility ($\text{m}^3/\text{mol}/\text{Pa}$) of a pure substance or endmember. |
| VK(ph,sp1,sp2,...) | Zero-order composition-dependent isothermal compressibility ($\text{m}^3/\text{mol}/\text{Pa}$) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase. |
| VK(ph,sp1,sp2,...i) | The ith -order composition-dependent isothermal compressibility ($\text{m}^3/\text{mol}/\text{Pa}$) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase. |
| WR(ph,sp) WR(ph,sp;0) | Standard Born function (J/mol) of a specific aqueous species in the AQUEOUS solution phase (always with a single sublattice) under the reference-state temperature and pressure. |

Technical Notes

In this section:

| | |
|----------------------------------------------------------------------|-----|
| Technical Note: Pipe or Redirect Output Data from Console Mode | 412 |
|----------------------------------------------------------------------|-----|

Technical Note: Pipe or Redirect Output Data from Console Mode

| | |
|--------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Audience: | Advanced Programmers and Users |
| OS: | Windows, Linux, or Mac |
| Application: | For users who want to pipe or redirect data from Thermo-Calc running a macro in Console Mode. |
| Command examples: | <p>Windows</p> <pre>Thermo-Calc.bat macro.tcm > results.log</pre> <p>Linux</p> <pre>Thermo-Calc.sh -E < macro.tcm > results.log</pre> <p>Mac</p> <pre>Thermo-Calc.command -E < macro.tcm > results.log</pre> |
| Command line definitions | |
| E | For Linux and Mac users, the Emacs style editing feature must be disabled (turned off) using the switch -E in order for redirection and piping to work correctly with Thermo-Calc. For Windows this flag is not necessary. |
| <> | Redirection commands. The direction of each arrow indicates the flow of data. For example in <code>./Console.sh -E < my_commands.tcm > results.log</code> , the contents of <code>my_commands.tcm</code> is used as input to the <code>Console.sh</code> script file and the resulting output is then written to <code>results.log</code> . |

Console Mode Examples

In this section:

| | |
|-----------------------------------------------------------------|-----|
| Thermo-Calc Console Mode Examples | 414 |
| Binary Phase Diagram Examples | 415 |
| Property Diagram Examples | 418 |
| Ternary Phase Diagram Examples | 423 |
| Multicomponent Phase Diagram Examples | 427 |
| Examples Calculating Thermodynamic and Related Quantities | 429 |
| Single Equilibrium Calculation Examples | 432 |
| Potential Diagram Example | 434 |
| Examples of Scheil-Gulliver Calculations | 434 |
| Example Calculating Chemical Ordering | 435 |
| Examples Using the Gibbs Energy System (GES) Module | 436 |
| Example Calculating the T0 Temperature | 439 |
| Examples Calculating Paraequilibrium | 439 |
| Example Using Functions and Variables | 441 |
| Example Using the PARROT and EDIT_EXPERIMENT Modules | 441 |
| Pourbaix Module Examples | 444 |
| Example Using the Tabulate Reaction (TAB) Module | 462 |
| Example Using the Reactor Module | 462 |
| Application Examples | 463 |

Thermo-Calc Console Mode Examples

There are many examples to examine and to help you learn Thermo-Calc in Console Mode. Some of the examples in the table below are included with specific sections, whereas some of the general examples are included (repeated) in more than one section.

Each topic has a brief description of the example and includes some or all of the commands used in the macros.

- ▶ ["About the Examples " on page 23](#)
- ▶ ["Opening Console Mode Macro Files" on page 20](#)



All the macro files and the outputs are also combined into one file that you can search and read. This is included with your installation as a PDF (go to **Help > Manuals folder > All Thermo-Calc Documentation** and open *Thermo-Calc Console Mode Example Macros*).

| Topic | TCEX Examples included |
|-----------------------------------------------------------------------------------------|-----------------------------------------------------|
| "Binary Phase Diagram Examples" on the next page | 1, 4, 13, 16, 17, 26, 31, 34, 50 |
| "Property Diagram Examples" on page 418 | 2, 8, 9, 11, 12, 22, 23, 25, 28, 29, 32, 41, 49, 50 |
| "Ternary Phase Diagram Examples" on page 423 | 3, 5, 14, 17, 19A, 19B, 21, 33, 37, 42, 43 |
| "Multicomponent Phase Diagram Examples" on page 427 | 6, 10, 23, 27 |
| "Examples Calculating Thermodynamic and Related Quantities" on page 429 | 2, 13, 14, 18, 22, 26, 34, 39, 51 |
| "Single Equilibrium Calculation Examples" on page 432 | 7, 18, 20 |
| " Potential Diagram Example" on page 434 | 35 |
| "Examples of Scheil-Gulliver Calculations" on page 434 | 15, 30A, 30B, 48, 54 |
| "Example Calculating Chemical Ordering" on page 435 | 16 |
| "Examples Using the Gibbs Energy System (GES) Module" on page 436 | 31, 38, 39, 49, 52 |
| "Example Calculating the T0 Temperature " on page 439 | 23 |
| "Examples Calculating Paraequilibrium" on page 439 | 23, 42, 43 |
| "Example Using Functions and Variables" on page 441 | 44 |
| "Example Using the PARROT and EDIT_EXPERIMENT Modules" on page 441 | 36 |
| "Pourbaix Module Examples" on page 444 | 40, 40A-E, 53 |

| Topic | TCEX Examples included |
|--------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| "Example Using the Tabulate Reaction (TAB) Module" on page 462 | 12 |
| "Example Using the Reactor Module" on page 462 | 24 |
| "Application Examples" on page 463 | 9 - Dew Point 10 - Continuous casting, preventing Cr_2O_3 clogging 11 - Gas oxidation of Cu_2S 20 - Adiabatic decompression in Geological system 24 - Silicon arc furnace 25 - Refinement of steel 27 - Chemical Vapour Deposition 28 - Materials design of a stainless steel 29 - Gas speciation 41 - Solubility product 44 - Proof strength calculated from empirical functions |

Binary Phase Diagram Examples

TCEX01 - CALCULATING THE BINARY Fe-C PHASE DIAGRAM

This example calculates the binary Fe-C phase diagram using the Binary module. The TCBIN database is used and included with your installation.

Some of the main commands used:

- ["LIST_EQUILIBRIUM" on page 171](#)
- ["LIST_STATUS" on page 172](#)
- ["LIST_CONDITIONS" on page 170](#)
- ["CHANGE_STATUS" on page 152](#)
- ["COMPUTE_EQUILIBRIUM" on page 156](#)
- ["SET_DIAGRAM_AXIS" on page 366](#)

-
- ["SET_TIELINE_STATUS" on page 375](#)
 - ["PLOT_DIAGRAM" on page 361](#)
 - ["SET_SCALING_STATUS" on page 374](#)
 - ["SET_LABEL_CURVE_OPTION" on page 369](#)
 - ["ADD_LABEL_TEXT" on page 352](#)
 - ["MODIFY_LABEL_TEXT" on page 360](#)

TCEX04 - CALCULATING THE Fe-Cr MISCIBILITY GAP

This example calculates the miscibility gap in the Fe-Cr system. The FEDEMO database is used and included with your installation.

These commands are used:

- ["SWITCH_DATABASE" on page 130](#)
- ["GET_DATA" on page 126](#)
- ["LIST_EQUILIBRIUM" on page 171](#)
- ["SET_AXIS_VARIABLE" on page 180](#)
- ["DEFINE_SYSTEM" on page 125](#)
- ["AMEND_PHASE_DESCRIPTION" on page 214](#)
- ["SET_CONDITION" on page 181](#)
- ["SAVE_WORKSPACES" on page 305](#)
- ["REJECT" on page 127](#)
- ["LIST_STATUS" on page 172](#)
- ["COMPUTE_EQUILIBRIUM" on page 156](#)
- ["SET_TIELINE_STATUS" on page 375](#)

TCEX13 - THE BINARY Al-Ti PHASE DIAGRAM AND ITS G CURVE

This example calculates an Al-Ti binary phase diagram and G curve using the BINARY module. The TCBIN database is used and included with your installation.

TCEX16 - SECOND ORDER TRANSITION OF THE Al-Fe SYSTEM

This example calculates the second order transition line in the Bcc field of the Al-Fe system.



This uses the SSOL database. A license is required to run the example.

These commands are of note and used in this example:

- ["REJECT" on page 127](#)
- ["RESTORE" on page 128](#)
- ["ADVANCED_OPTIONS" on page 135](#)
- ["SET_SCALING_STATUS" on page 374](#)
- ["DEFINE_SYSTEM" on page 125](#)
- ["MAKE_EXPERIMENTAL_DATAFILE" on page 360](#)
- ["LIST_EQUILIBRIUM" on page 171](#)
- ["APPEND_EXPERIMENTAL_DATA" on page 353](#)
- ["STEP_WITH_OPTIONS" on page 188](#)

TCEX17 - THE PSEUDO-BINARY SYSTEM - CaO-SiO_2

This example calculates the pseudo-binary system CaO-SiO_2 using the OXDEMO database, which is included with your installation.

The oxide demo (Oxdemo) database can be used both for pseudo-binary systems like the one in this case, CaO-SiO_2 , or for full ternary systems like Ca-Fe-O .

These commands are of note and used in this example:

- ["LIST_SYSTEM" on page 127](#)
- ["REJECT" on page 127](#) and ["RESTORE" on page 128](#)
- ["AMEND_PHASE_DESCRIPTION" on page 214](#)
- ["LIST_STATUS" on page 172](#)
- ["DEFINE_COMPONENTS" on page 160](#)
- ["SET_CONDITION" on page 181](#)
- ["COMPUTE_EQUILIBRIUM" on page 156](#) and ["LIST_EQUILIBRIUM" on page 171](#)

TCEX26 - THE AS-GA PHASE DIAGRAM: PLOTTING THE PARTIAL PRESSURES OF A GAS SPECIES

This example uses the PG35 Binary Semi-Conductors database and is an example of plotting

the partial pressures of a gas species along the solubility lines in the As-Ga phase diagram. The calculation makes it possible to monitor the input gases to a process of depositing solid As-Ga.

These commands are of note and used in this example:

- ["REJECT" on page 127](#)
- ["RESTORE" on page 128](#)
- ["SET_DIAGRAM_AXIS" on page 366](#)
- ["SET_SCALING_STATUS" on page 374](#)
- ["SET_AXIS_TEXT_STATUS" on page 363](#)
- ["SET_LABEL_CURVE_OPTION" on page 369](#)

TCEX31 - USING THE GES MODULE TO CALCULATE CVM

Using the Gibbs Energy System (GES) module, this example calculates the CVM and compares it with the sublattices of a fictitious A B system. You also learn how to overlay diagrams from two calculations.

These GES commands are of note and used in this example:

- ["ENTER_ELEMENT" on page 221](#)
- ["ENTER_SPECIES" on page 230](#)
- ["ENTER_SYMBOL" on page 231](#)
- ["ENTER_PHASE" on page 228](#)
- ["ENTER_PARAMETER" on page 268](#)
- ["LIST_PHASE_DATA" on page 272](#)

TCEX34 - THE AL-ZN PHASE DIAGRAM AND ITS G CURVE

This example uses the BINARY module to calculate the phase diagram and G curves in the Al-Zn system. It uses the TCBIN database included with your installation.

Property Diagram Examples

TCEX02 - PLOTTING THERMODYNAMIC FUNCTIONS

This example shows how to plot thermodynamic functions in unary, binary and ternary

systems. It also involves working with partial derivatives and partial quantities.



This uses the SSOL database. A license is required to run the example.

These commands are used:

| | | |
|-----------------------------------------------|-------------------------------------------------------|------------------------------------------------------|
| "GOTO_MODULE" on page 113 | "GET_DATA" on page 126 | "SET_CONDITION" on page 181 |
| "SWITCH_DATABASE" on page 130 | "AMEND_PHASE_DESCRIPTION" on page 214 | "LIST_EQUILIBRIUM" on page 171 |
| "DEFINE_SYSTEM" on page 125 | "COMPUTE_EQUILIBRIUM" on page 156 | "SET_AXIS_VARIABLE" on page 180 |
| "SAVE_WORKSPACES" on page 305 | "STEP_WITH_OPTIONS" on page 188 | "SET_DIAGRAM_AXIS" on page 366 |
| "ENTER_SYMBOL" on page 167 | "PLOT_DIAGRAM" on page 361 | "SET_LABEL_CURVE_OPTION" on page 369 |
| "REJECT" on page 127 | "RESTORE" on page 128 | "LIST_SYSTEM" on page 127 |
| "LIST_STATUS" on page 172 | "CHANGE_STATUS" on page 152 | "SHOW_VALUE" on page 188 |
| "SET_INTERACTIVE" on page 119 | | |

TCEx08 - PROPERTY DIAGRAMS FOR A HIGH SPEED STEEL

This example shows how to calculate property diagrams for a high speed steel i.e. phase fraction plots, activity vs temperature, and so forth.



This uses the TCFE database. A license is required to run the example.

These commands are of note and used in this example:

- ["DEFINE_DIAGRAM" on page 161](#)
- ["DEFINE_ELEMENTS" on page 124](#)
- ["AMEND_PHASE_DESCRIPTION" on page 214](#)

-
- ["REINITIATE_PLOT_SETTINGS" on page 362](#)

TCEX09 - CALCULATING A DEW POINT WITH THE POLY3 MODULE

This is an example calculating the dew point in the POLY3 module. The SUBDEMO database is used and included with your installation.

The STEP_WITH_OPTIONS and MAP commands are of note and used in this example.

TCEX11 - OXIDATION OF CU₂S WITH AN H₂O/O₂ GAS MIXTURE

This example demonstrates the oxidation of Cu₂S with an H₂O/O₂ gas mixture. Thermo-Calc is used to find the optimum O/H ratio (i.e. oxygen potential) as certain oxygen potential values can desulphurize Cu₂S without forming copper oxides.

In Thermo-Calc, the problem reduces to perform equilibria calculations in a Cu-S-H-O system. The amounts of the components should be kept to correct ratio corresponding to Cu₂S and H₂O using a command SET_INPUT_AMOUNTS in POLY3. Initially, O/H = 0.5 is given. Optimum O/H ratio is calculated with the desired calculation conditions. For example, to simulate one phase disappearing, you can FIX the phase with zero amount.

The *tcex11.TDB* file is used to access data and this is included with your installation.

These commands are of also of note and used in this example:

- ["SET_NUMERICAL_LIMITS" on page 184](#)
- ["SET_REFERENCE_STATE" on page 185](#)
- ["SHOW_VALUE" on page 188](#)

TCEX12 - TABULATION OF THERMODYNAMIC DATA FOR REACTIONS

This example shows a number of independent cases using the TABULATE_REACTION (TAB) module to tabulate thermodynamic data for reactions.



This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- ["TABULATE_REACTION" on page 333](#)
- ["DEFINE_SPECIES" on page 124](#)
- ["ENTER_FUNCTION" on page 222](#)

-
- ["QUICK_EXPERIMENTAL_PLOT" on page 362](#)
 - ["SET_SCALING_STATUS" on page 374](#)
 - ["LIST_SUBSTANCES" on page 324](#)
 - ["TABULATE_SUBSTANCE" on page 336](#)

TCEX22 - CALCULATING AN ADIABATIC FLAME TEMPERATURE

This example examines a heat balance when C_3H_8 is burned in oxygen by calculating the adiabatic flame temperature.



This uses the SSUB database. A license is required to run the example.

TCEX23 - CALCULATING A PARAEQUILIBRIUM AND THE T0 TEMPERATURE IN A LOW ALLOYED STEEL

This example calculates a paraequilibrium and the T0 temperature in a low alloyed steel.



This uses the TCFE database. A license is required to run the example.

TCEX25 - SIMULATING THE REFINEMENT OF STEEL

This example is based on a typical steel refining process. Raw iron used to produce steel usually has high carbon and silicon content, which is why oxygen is blown into the furnace to burn off carbon. Lime (CaO) is added to form a slag with silica, and the slag can be removed. Alloying elements, such as Mn, Ni, Cr and V are added to produce the desired steel. Since the reaction between O and C increases the temperature, scrap iron is added to keep the temperature constant (it is assumed the furnace is isolated and no heat is lost to the environment).

This example simulates blowing oxygen into a liquid steel of one metric ton (1e6 grams) with 4 w/o C, 2 w/o Si and 1 w/o Mn. 100 moles of CaO (equivalent to 5.6 kg) is added. Keeping the enthalpy constant is the way to simulate the isolation of the furnace. The oxygen reacts with carbon and increases the temperature. After blowing a certain amount of oxygen, scrap iron is added to keep the temperature constant.



This uses the SLAG database. A license is required to run the example.

TCEX28 - PITTING RESISTANCE EQUIVALENCE (PRE) FOR A DUPLEX STAINLESS STEEL

This example calculates the Pitting Resistance Equivalence (PRE) for a duplex stainless steel.



This uses the TCFE database. A license is required to run the example.

These commands are of note and used in this example:

- ["REJECT" on page 127](#)
- ["RESTORE" on page 128](#)
- ["DEFINE_ELEMENTS" on page 124](#)
- ["AMEND_PHASE_DESCRIPTION" on page 214](#)
- ["EVALUATE_FUNCTIONS" on page 170](#)
- ["SET_START_CONSTITUTION" on page 187](#)

TCEX29 - CALCULATING THE SPECIATION OF A GAS

This example shows how to calculate the speciation of a gas.



This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- ["SET_INPUT_AMOUNTS" on page 183](#)
- ["LIST_CONDITIONS" on page 170](#)
- ["SET_CONDITION" on page 181](#)

TCEX32 - CALCULATING OXIDE LAYERS ON STEEL

This example calculates oxide layers on a steel and shows how to append databases.



This uses the TCFE and SSUB databases. These licenses are required to run the example.

These commands are of note and used in this example:

- ["SET_START_CONSTITUTION" on page 187](#)
- ["SET_REFERENCE_STATE" on page 185](#)

-
- ["APPEND_DATABASE" on page 123](#)

TCEX41 - CALCULATING A SOLUBILITY PRODUCT

Calculation of a solubility product.



This uses the TCFE database. A license is required to run the example.

These commands are of note and used in this example:

- ["DEFINE_ELEMENTS" on page 124](#)
- ["REINITIATE_PLOT_SETTINGS" on page 362](#)
- ["SET_DIAGRAM_AXIS" on page 366](#)

TCEX49 - QUASICHEMICAL MODEL USING THE GIBBS ENERGY SYSTEM (GES) MODULE

This example shows how to enter parameters for a FACT quasichemical liquid model and how to calculate the sulfur activity using the GIBBS_ENERGY_SYSTEM (GES) module commands.

These commands are of note and used in this example:

- ["ENTER_ELEMENT" on page 221](#)
- ["ENTER_SYMBOL" on page 231](#)
- ["AMEND_ELEMENT_DATA" on page 204](#)
- ["ENTER_PARAMETER" on page 268](#)
- ["ENTER_SPECIES" on page 230](#)
- ["SET_REFERENCE_STATE" on page 185](#)
- ["SHOW_VALUE" on page 188](#)

Ternary Phase Diagram Examples

TCEX03 - CALCULATING AN ISOTHERMAL SECTION WITH THE TERNARY MODULE

This example calculates an isothermal section using the Ternary module. The FEDEMO database is used and included with your installation.

These commands are used:

-
- ["AMEND_PHASE_DESCRIPTION" on page 214](#)
 - ["ADD_LABEL_TEXT" on page 352](#)
 - ["PLOT_DIAGRAM" on page 361](#)
 - ["SET_DIAGRAM_AXIS" on page 366](#); ["SET_DIAGRAM_TYPE" on page 368](#); and ["SET_AXIS_TYPE" on page 364](#)
 - ["SET_REFERENCE_STATE" on page 185](#)
 - ["CHANGE_STATUS" on page 152](#)
 - ["SET_SCALING_STATUS" on page 374](#)

TCEX05 - CALCULATING A VERTICAL SECTION IN THE AL-CU-SI SYSTEM

This example calculates a vertical section in the Al-Cu-Si system and of a vertical section from Al to 10% Cu₂Si. The ALDEMO database is used and included with your installation.

TCEX14 - VARIATIONS IN SOLIDIFICATION OF AN AL-MG-SI ALLOY

This example calculates the heat and heat capacity variations during solidification of an Al-Mg-Si alloy. The ALDEMO database is used and included with your installation.

These commands are of note and used in this example:

- ["LIST_SYSTEM" on page 127](#)
- ["LIST_CONDITIONS" on page 170](#)
- ["SET_AXIS_TEXT_STATUS" on page 363](#)

TCEX17 - THE PSEUDO-BINARY SYSTEM - CAO-SIO2

This example calculates the pseudo-binary system CaO-SiO₂ using the OXDEMO database, which is included with your installation.

The oxide demo (Oxdemo) database can be used both for pseudo-binary systems like the one in this case, CaO-SiO₂, or for full ternary systems like Ca-Fe-O.

These commands are of note and used in this example:

- ["LIST_SYSTEM" on page 127](#)
- ["REJECT" on page 127](#) and ["RESTORE" on page 128](#)
- ["AMEND_PHASE_DESCRIPTION" on page 214](#)

-
- ["LIST_STATUS" on page 172](#)
 - ["DEFINE_COMPONENTS" on page 160](#)
 - ["SET_CONDITION" on page 181](#)
 - ["COMPUTE_EQUILIBRIUM" on page 156](#) and ["LIST_EQUILIBRIUM" on page 171](#)

TCEX19A AND TCEX19B - MAPPING OF UNIVARIANT EQUILIBRIA WITH THE LIQUID IN AL-CU-SI

- Part A. Step-by-step calculation using the POLY3 module.
- Part B. Using the TERNARY module, you can get the information on invariant reactions, such as temperature and compositions.

These commands are of note and used in these examples:

- ["DEFINE_SYSTEM" on page 125](#)
- ["GET_DATA" on page 126](#)
- ["AMEND_PHASE_DESCRIPTION" on page 214](#)
- ["SET_CONDITION" on page 181](#) and ["LIST_CONDITIONS" on page 170](#)
- ["ADVANCED_OPTIONS" on page 135](#)
- ["SAVE_WORKSPACES" on page 305](#) and ["READ_WORKSPACES" on page 241](#)
- ["APPEND_EXPERIMENTAL_DATA" on page 353](#)
- ["MAKE_EXPERIMENTAL_DATAFILE" on page 360](#)

TCEX21 - CALCULATING A TERNARY ISOTHERM IN Fe-Cr-Ni

This example calculates a ternary isotherm in Fe-Cr-Ni with a user-defined database included with the example in the file named *tcex21.TDB*.

These commands are of note and used in this example:

- ["DEFINE_SYSTEM" on page 125](#)
- ["GET_DATA" on page 126](#)
- ["SET_CONDITION" on page 181](#)
- ["SET_DIAGRAM_TYPE" on page 368](#)

TCEX33 - AN Fe-Cr-C ISOPLETH

This example is a benchmark calculation of an isopleth in the Fe-Cr-C system. The FEDemo database is used and included with your installation.

TCEX37 - CALCULATING AN ISOTHERMAL SECTION IN CONSOLE MODE

This example shows how to use command lines to enter and calculate an isothermal section using the POLY3 module. The FEDEMO database is used and included with your installation.

TCEX42 - PARAEQUILIBRIUM CALCULATION - FORMATION OF PARA-PEARLITE - ISOPLETH



This uses the TCFE database. A license is required to run the example.

This example uses an Fe-Mn-C system at 2.5%Mn Mass u-fraction to show a paraequilibrium calculation where there is formation of para-pearlite. It is an isopleth calculation and shows the STEP_WITH_OPTIONS command using the Paraequilibrium option.

TCEX43 - PARAEQUILIBRIUM CALCULATION - FORMATION OF PARA-PEARLITE - ISOTHERMAL



This uses the TCFE database. A license is required to run the example.

This example uses an Fe-Mn-C system at 700 C to show a paraequilibrium calculation where there is formation of para-pearlite. It is an isothermal calculation and shows the STEP_WITH_OPTIONS command using the Paraequilibrium option.

Multicomponent Phase Diagram Examples

TCEX06 - AN ISOPLETH IN LOW ALLOYED FE-MN-SI-CR-NI-C STEEL

This example calculates a multicomponent phase diagram using the DEFINE_MATERIAL command in POLY and the TCFE steel database. The material contains 1.5 %Cr + 0.4 %Mn + 3.5 %Ni + 0.3 %Si and 1 %C (by weight). These conditions and the temperature are set by the DEFINE_MATERIAL command.

After the first equilibrium results, a phase diagram is calculated with one axis variable as temperature and the other as the carbon content.



This uses the TCFE database. A license is required to run the example.

TCEX10 - PREVENTING CR₂O₃ CLOGGING IN A CONTINUOUS CASTING PROCESS

The example calculates an equilibrium with suspended or dormant phases and shows how to avoid Cr_2O_3 clogging in a continuous casting process.



This uses the SLAG database. A license is required to run the example.

The origin of this example is that a manufacturer wanted to increase the Cr content of a material from 18 to 25 weight percent but the continuous casting of this material was problematic because solid Cr_2O_3 was formed.

Using Thermo-Calc to calculate the equilibria in the steel/slag system, a simple correction was found: modify the Mn or Si content to decrease the oxygen potential. In Thermo-Calc, you can FIX a phase with zero amount to simulate how to avoid forming this phase. You then release one of the conditions, usually one of the compositions, and this composition is determined by the equilibrium calculation.

These commands are used:

| | | |
|------------------------------------------------|-------------------------------------------------------|----------------------------------------------------|
| "DEFINE_SYSTEM" on page 125 | "AMEND_PHASE_DESCRIPTION" on page 214 | "GET_DATA" on page 126 |
| "SET_CONDITION" on page 181 | "LIST_CONDITIONS" on page 170 | "LIST_STATUS" on page 172 |
| "CHANGE_STATUS" on page 152 | "COMPUTE_EQUILIBRIUM" on page 156 | "SET_NUMERICAL_LIMITS" on page 184 |
| "LIST_EQUILIBRIUM" on page 171 | "SET_REFERENCE_STATE" on page 185 | "SHOW_VALUE" on page 188 |

TCEx23 - CALCULATING A PARAEQUILIBRIUM AND THE T₀ TEMPERATURE IN A LOW ALLOYED STEEL

This example calculates a paraequilibrium and the T₀ temperature in a low alloyed steel.



This uses the TCFE database. A license is required to run the example.

TCEx27 - CALCULATING CHEMICAL VAPOR DEPOSITIONS (CVD)

This example calculates the chemical vapor deposition (CVD).



This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- ["DEFINE_COMPONENTS" on page 160](#)
- ["SET_CONDITION" on page 181](#)
- ["ADD_INITIAL_EQUILIBRIUM" on page 133](#)
- ["LIST_AXIS_VARIABLE" on page 170](#)
- ["LIST_INITIAL_EQUILIBRIA" on page 172](#)

Examples Calculating Thermodynamic and Related Quantities

TCEx02 - PLOTTING THERMODYNAMIC FUNCTIONS

This example shows how to plot thermodynamic functions in unary, binary and ternary systems. It also involves working with partial derivatives and partial quantities.



This uses the SSOL database. A license is required to run the example.

These commands are used:

| | | |
|-----------------------------------------------|-------------------------------------------------------|------------------------------------------------------|
| "GOTO_MODULE" on page 113 | "GET_DATA" on page 126 | "SET_CONDITION" on page 181 |
| "SWITCH_DATABASE" on page 130 | "AMEND_PHASE_DESCRIPTION" on page 214 | "LIST_EQUILIBRIUM" on page 171 |
| "DEFINE_SYSTEM" on page 125 | "COMPUTE_EQUILIBRIUM" on page 156 | "SET_AXIS_VARIABLE" on page 180 |
| "SAVE_WORKSPACES" on page 305 | "STEP_WITH_OPTIONS" on page 188 | "SET_DIAGRAM_AXIS" on page 366 |
| "ENTER_SYMBOL" on page 167 | "PLOT_DIAGRAM" on page 361 | "SET_LABEL_CURVE_OPTION" on page 369 |
| "REJECT" on page 127 | "RESTORE" on page 128 | "LIST_SYSTEM" on page 127 |
| "LIST_STATUS" on page 172 | "CHANGE_STATUS" on page 152 | "SHOW_VALUE" on page 188 |

| | | |
|-----------------------------------------------|--|--|
| "SET_INTERACTIVE" on page 119 | | |
|-----------------------------------------------|--|--|

TCEX13 - THE BINARY AL-TI PHASE DIAGRAM AND ITS G CURVE

This example calculates an Al-Ti binary phase diagram and G curve using the BINARY module. The TCBIN database is used and included with your installation.

TCEX14 - VARIATIONS IN SOLIDIFICATION OF AN AL-MG-SI ALLOY

This example calculates the heat and heat capacity variations during solidification of an Al-Mg-Si alloy. The ALDEMO database is used and included with your installation.

These commands are of note and used in this example:

- ["LIST_SYSTEM" on page 127](#)
- ["LIST_CONDITIONS" on page 170](#)
- ["SET_AXIS_TEXT_STATUS" on page 363](#)

TCEX18 - A3 TEMPERATURE OF A STEEL

This example calculates the A3 temperature of a steel and examines the influence of each alloying element on this temperature.

A3 temperature is the temperature where ferrite starts to form from austenite. You can easily read A3 from an Fe-C phase diagram. However, for complex multicomponent steels no simple diagram can be used. Using POLY, it is easy to find out the influence of each alloying element on the A3 temperature. This information is useful if you want to modify the compositions of a steel but keep A3 unchanged.



This uses the TCFE database. A license is required to run the example.

These commands are of note and used in this example:

- ["DEFINE_ELEMENTS" on page 124](#)
- ["AMEND_PHASE_DESCRIPTION" on page 214](#)
- ["COMPUTE_TRANSITION" on page 158](#)
- ["DEFINE_MATERIAL" on page 163](#)

-
- ["ENTER_SYMBOL" on page 167](#)
 - ["SHOW_VALUE" on page 188](#)

TCEX22 - CALCULATING AN ADIABATIC FLAME TEMPERATURE

This example examines a heat balance when C_3H_8 is burned in oxygen by calculating the adiabatic flame temperature.



This uses the SSUB database. A license is required to run the example.

TCEX26 - THE AS-GA PHASE DIAGRAM: PLOTTING THE PARTIAL PRESSURES OF A GAS SPECIES

This example uses the PG35 Binary Semi-Conductors database and is an example of plotting the partial pressures of a gas species along the solubility lines in the As-Ga phase diagram. The calculation makes it possible to monitor the input gases to a process of depositing solid As-Ga.

These commands are of note and used in this example:

- ["REJECT" on page 127](#)
- ["RESTORE" on page 128](#)
- ["SET_DIAGRAM_AXIS" on page 366](#)
- ["SET_SCALING_STATUS" on page 374](#)
- ["SET_AXIS_TEXT_STATUS" on page 363](#)
- ["SET_LABEL_CURVE_OPTION" on page 369](#)

TCEX34 - THE AL-ZN PHASE DIAGRAM AND ITS G CURVE

This example uses the BINARY module to calculate the phase diagram and G curves in the Al-Zn system. It uses the TCBIN database included with your installation.

TCEX39 - CALCULATING REVERSIBLE CARNOT CYCLES OF A HEAT ENGINE

This example shows how to calculate the reversible Carnot cycle of a heat engine using one mole of an ideal gas with two fictitious species A and A2. The GES, POLY3 and POST modules are used, as well as the SUBDEMO database, which is included with your installation.

One application of the Second Law is to the efficiencies of heat engines, pumps and refrigerators. Whenever there is a difference of temperature, work can be produced - the principle of heat engines. The Gibbs energy also enables the prediction of the maximum work that a process may achieve. The goal of this example is to help relate the results to different thermodynamic quantities.

These commands are of note and used in this example:

- ["REINITIATE" on page 242](#)
- ["ENTER_PARAMETER" on page 268](#)
- ["ENTER_SPECIES" on page 230](#)
- ["SET_PLOT_FORMAT" on page 370](#)
- ["ENTER_PHASE" on page 228](#)

TCEX51 - CALCULATION OF MOLAR VOLUME, THERMAL EXPANSIVITY AND DENSITY

This example uses the POLY3 module to calculate the molar volume, thermal expansivity and density of the FCC_A1, BCC_A2 LIQUID and liquid phases of C-Fe.



This uses the TCFE database. A license is required to run the example.

Single Equilibrium Calculation Examples

TCEX07 - SINGLE EQUILIBRIA IN LOW ALLOYED FE-MN-SI-CR-NI-C STEEL

This example shows how to calculate a single equilibria in a low alloyed Fe-Mn-Si-Cr-Ni-C steel. There are two common ways to perform a single equilibrium calculation:

- Get data from a database, then in POLY use SET_CONDITION and COMPUTE_EQUILIBRIUM.
- Go directly to POLY and use DEFINE_MATERIAL.

The COMPUTE_TRANSITION command is also used to determine the temperature or composition where one phase forms or disappears. It is the same as the CHANGE_STATUS → SET_CONDITION → COMPUTE_EQUILIBRIUM sequence of commands.

A STEP_WITH_OPTIONS command using the option *normal* is also used in addition to the other commands that should be becoming more familiar as you work through the examples.



This uses the TCFE database. A license is required to run the example.

TCEX18 - A3 TEMPERATURE OF A STEEL

This example calculates the A3 temperature of a steel and examines the influence of each alloying element on this temperature.

A3 temperature is the temperature where ferrite starts to form from austenite. You can easily read A3 from an Fe-C phase diagram. However, for complex multicomponent steels no simple diagram can be used. Using POLY, it is easy to find out the influence of each alloying element on the A3 temperature. This information is useful if you want to modify the compositions of a steel but keep A3 unchanged.



This uses the TCFE database. A license is required to run the example.

These commands are of note and used in this example:

- ["DEFINE_ELEMENTS" on page 124](#)
- ["AMEND_PHASE_DESCRIPTION" on page 214](#)
- ["COMPUTE_TRANSITION" on page 158](#)
- ["DEFINE_MATERIAL" on page 163](#)
- ["ENTER_SYMBOL" on page 167](#)
- ["SHOW_VALUE" on page 188](#)

TCEX20 - ADIABATIC DECOMPRESSION IN A GEOLOGICAL SYSTEM

This example calculates the adiabatic decompression in a geological system using the geochemical database. The database is included with the file named PGEO.TDB, which is in the same folder as this example.

These commands are of note and used in this example:

- ["DEFINE_SYSTEM" on page 125](#)
- ["DEFINE_COMPONENTS" on page 160](#)
- ["SET_INPUT_AMOUNTS" on page 183](#)
- ["LIST_CONDITIONS" on page 170](#)
- ["SET_CONDITION" on page 181](#)

-
- ["SHOW_VALUE" on page 188](#)

Potential Diagram Example

TCEX35 - CALCULATING A POTENTIAL DIAGRAM

This example uses the POTENTIAL module to calculate a potential diagram. Note that there are no commands for this module, you just follow the prompts. The SUBDEMO database is used and included with your installation.

Examples of Scheil-Gulliver Calculations

- ▶ ["About the Scheil-Gulliver Solidification Simulations " on page 72](#)

TCEX15 - SIMULATING THE SOLIDIFICATION OF A CR-NI ALLOY WITH THE SCHEIL MODULE

This is an example of a solidification simulation of a Cr-Ni alloy. There is no back diffusion in the solid, i.e. Scheil-Gulliver model is used.



This uses the TCFE database. A license is required to run the example.

These commands are of note and used in this example:

- ["START_WIZARD" on page 250](#)
- ["COMPUTE_TRANSITION" on page 158](#)
- ["ADD_INITIAL_EQUILIBRIUM" on page 133](#)
- ["ENTER_SYMBOL" on page 167](#)
- ["ADVANCED_OPTIONS" on page 135](#)
- ["STEP_WITH_OPTIONS" on page 188](#)
- ["MAKE_EXPERIMENTAL_DATAFILE" on page 360](#)
- ["CHANGE_STATUS" on page 152](#)

TCEX30A AND 30B - SCHEIL CALCULATION FOR AN AL-4MG-2SI-2CU ALLOY

- ▶ ["The Equilibrium Calculation Module \(POLY3\)" on page 39](#) and ["About the Scheil-Gulliver Solidification Simulations " on page 72](#)

These examples show two ways to do a Scheil calculation for an Al-4Mg-2Si-2Cu alloy. In part A, you use the POLY3 module and the STEP_WITH_OPTIONS command with an EVALUATE option. Then in part B you use the SCHEIL module commands to do the same thing. Data from the COST2 database is used and included with the example in the file named *tcex30_cost2.TDB*.

TCEX48 - SCHEIL SOLIDIFICATION WITH C BACK DIFFUSION

This is an example of Scheil solidification with C back diffusion in solid phases. The results are compared between a simple Scheil and equilibrium calculation. The FEDEMO database is used.

TCEX54 - SCHEIL SOLIDIFICATION OF AN AL-2.1Cu-1Si ALLOY INCLUDING BACK DIFFUSION

This is an example of a solidification simulation of a Al-2.1Cu-1Si alloy. The back diffusion option in the Scheil module is used, i.e. there is back diffusion in the primary phase. The example uses both the thermodynamic ALDEMO and mobility MALDEMO demo databases included with your installation.

Example Calculating Chemical Ordering

TCEX16 - SECOND ORDER TRANSITION OF THE AL-FE SYSTEM

This example calculates the second order transition line in the Bcc field of the Al-Fe system.



This uses the SSOL database. A license is required to run the example.

These commands are of note and used in this example:

- ["REJECT" on page 127](#)
- ["RESTORE" on page 128](#)
- ["ADVANCED_OPTIONS" on page 135](#)
- ["SET_SCALING_STATUS" on page 374](#)
- ["DEFINE_SYSTEM" on page 125](#)
- ["MAKE_EXPERIMENTAL_DATAFILE" on page 360](#)
- ["LIST_EQUILIBRIUM" on page 171](#)
- ["APPEND_EXPERIMENTAL_DATA" on page 353](#)

-
- ["STEP_WITH_OPTIONS" on page 188](#)

Examples Using the Gibbs Energy System (GES) Module

TCEx31 - USING THE GES MODULE TO CALCULATE CVM

Using the Gibbs Energy System (GES) module, this example calculates the CVM and compares it with the sublattices of a fictitious A B system. You also learn how to overlay diagrams from two calculations.

These GES commands are of note and used in this example:

- ["ENTER_ELEMENT" on page 221](#)
- ["ENTER_SPECIES" on page 230](#)
- ["ENTER_SYMBOL" on page 231](#)
- ["ENTER_PHASE" on page 228](#)
- ["ENTER_PARAMETER" on page 268](#)
- ["LIST_PHASE_DATA" on page 272](#)

TCEx38 - CALCULATING THE MORRAL "ROSE"

This example uses the Gibbs energy system (GES) module to calculate the Morral rose, which are miscibility gaps.

These commands are of note and used in this example:

- ["REINITIATE" on page 242](#)
- ["ENTER_ELEMENT" on page 221](#)
- ["AMEND_ELEMENT_DATA" on page 204](#)
- ["ENTER_PARAMETER" on page 268](#)
- ["ENTER_PHASE" on page 228](#)

TCEx39 - CALCULATING REVERSIBLE CARNOT CYCLES OF A HEAT ENGINE

This example shows how to calculate the reversible Carnot cycle of a heat engine using one mole of an ideal gas with two fictitious species A and A2. The GES, POLY3 and POST modules

are used, as well as the SUBDEMO database, which is included with your installation.

One application of the Second Law is to the efficiencies of heat engines, pumps and refrigerators. Whenever there is a difference of temperature, work can be produced - the principle of heat engines. The Gibbs energy also enables the prediction of the maximum work that a process may achieve. The goal of this example is to help relate the results to different thermodynamic quantities.

These commands are of note and used in this example:

- ["REINITIATE" on page 242](#)
- ["ENTER_PARAMETER" on page 268](#)
- ["ENTER_SPECIES" on page 230](#)
- ["SET_PLOT_FORMAT" on page 370](#)
- ["ENTER_PHASE" on page 228](#)

TCEX49 - QUASICHEMICAL MODEL USING THE GIBBS ENERGY SYSTEM (GES) MODULE

This example shows how to enter parameters for a FACT quasichemical liquid model and how to calculate the sulfur activity using the GIBBS_ENERGY_SYSTEM (GES) module commands.

These commands are of note and used in this example:

- ["ENTER_ELEMENT" on page 221](#)
- ["ENTER_SYMBOL" on page 231](#)
- ["AMEND_ELEMENT_DATA" on page 204](#)
- ["ENTER_PARAMETER" on page 268](#)
- ["ENTER_SPECIES" on page 230](#)
- ["SET_REFERENCE_STATE" on page 185](#)
- ["SHOW_VALUE" on page 188](#)

TCEX52 - CHANGING THE EXCESS MODELS FOR INTERACTION PARAMETERS IN A SOLUTION PHASE

-  ["Solution Models in the GIBBS \(GES\) Module" on page 207](#)

This example shows how to change the excess models for binary and ternary interactions in a solution phase, either

-
- through direct interactive amendments of phase descriptions within the GIBBS_ENERGY_SYSTEM (GES) module, or
 - enforced by specific type-definitions given in a database file retrieved by the DATABASE_RETRIEVAL module (also called the TDB module).

For binary excess models, the example changes it from the default *R-K model* to a *Mixed-Excess-Model*. The phase has to be a substitutional phase in this case.

For ternary extrapolation models, the example changes it from the default *R-K-M model* to a *Toop_Kohler model*.

Notes related to the example

The following is included in the macro file as part of the instructions but may be of use to new users:

Amending the binary excess model

The default binary excess model is the Redlich-Kister Model for all the three associated binary interaction pairs (A-B, A-C and B-C) in the substitutional LIQUID solution phase (without sublattice) that consists of three elements (A, B and C).

Before changing this default binary excess model for the ternary LIQUID solution phase, one must have already entered the G parameters (for standard Gibbs energies of all pure end-members) and L parameters (for binary R-K excess interaction energies), as shown in the example.

In this particular example, we want to change from the default R-K binary excess model to the Mixed-Excess-Model (with three different binary excess models, namely Legendre, Polynom and Redlich-Kister models, applied to the A-B, A-C and B-C binaries, respectively), as demonstrated below:

For the A-B interaction, the Legendre binary excess model should be used (rather than the default Redlich-Kister Model), with the first species (i.e. A) as the independent constituent and the second species (i.e. B) as the dependent constituent, while the L parameters for the A-B interaction shall remain the same as those handled by the R-K model.

For the A-C interaction, the Polynom binary excess model should be used (rather than the default Redlich-Kister Model), with the second species (i.e. C) as the independent constituent and the first species (i.e. A) as the dependent constituent, while the L parameters for the A-C interaction shall remain the same as those handled by the R-K model.

Amending the ternary extrapolation model

The default ternary excess model is the Redlich-Kister_Muggianu Model (i.e., the MUGGIANU_RESTOR method for ternary extrapolation based on binary parameters) for the associated ternary interaction terms; when no ternary L parameter is entered for that, such a default Redlich-Kister_Muggianu Model is thus to be used for extrapolation from binary excess energies to ternary interactions in the substitutional LIQUID solution phase (without sublattice) that consists of three elements (A, B and C).

However, in this particular example as illustrated in the following, we shall change from this default R-K-M ternary excess model to the TOOP-KOHLER method for the ternary extrapolation method, with the species C as the Toop constituent, while the species A and B as the Kohler constituents (entering A and B, or B and A, as the basis constituent and first interacting constituent). This will implicitly enforce that, during the ternary extrapolation, only the A-B binary interaction parameters are utilized in accordance with the Kohler ternary extrapolation formula for A-B-C ternary interaction, while any other binary interaction parameters used in line with the Toop-Kohler ternary extrapolation formula (for the A-C-B and B-C-A ternary interactions). This makes the extrapolated ternary excess interaction terms different from those handled either by the default MUGGIANU_RESTOR method or by the alternative KOHLER-ALL method.

Note that only when all the relevant binary excess energies in a ternary system are treated by the default Redlich-Kister Model (i.e., the Mixed-Excess-Model should have not been used), the MUGGIANU_RESTOR method for ternary extrapolations is equivalent to the Redlich-Kister_Muggianu Model, or the KOHLER-ALL method to the Redlich-Kister_Kohler Model.

Example Calculating the T0 Temperature

TCEX23 - CALCULATING A PARAEQUILIBRIUM AND THE T0 TEMPERATURE IN A LOW ALLOYED STEEL

This example calculates a paraequilibrium and the T0 temperature in a low alloyed steel.



This uses the TCFE database. A license is required to run the example.

Examples Calculating Paraequilibrium

TCEX23 - CALCULATING A PARAEQUILIBRIUM AND THE T0 TEMPERATURE IN A LOW ALLOYED STEEL

This example calculates a paraequilibrium and the T0 temperature in a low alloyed steel.



This uses the TCFE database. A license is required to run the example.

TCEX42 - PARAEQUILIBRIUM CALCULATION - FORMATION OF PARA-PEARLITE - ISOPLETH



This uses the TCFE database. A license is required to run the example.

This example uses an Fe-Mn-C system at 2.5%Mn Mass u-fraction to show a paraequilibrium calculation where there is formation of para-pearlite. It is an isopleth calculation and shows the STEP_WITH_OPTIONS command using the Paraequilibrium option.

TCEX43 - PARAEQUILIBRIUM CALCULATION - FORMATION OF PARA-PEARLITE - ISOTHERMAL



This uses the TCFE database. A license is required to run the example.

This example uses an Fe-Mn-C system at 700 C to show a paraequilibrium calculation where there is formation of para-pearlite. It is an isothermal calculation and shows the STEP_WITH_OPTIONS command using the Paraequilibrium option.

Example Using Functions and Variables

TCEX44 - EXPLORING VARIABLES AND FUNCTIONS

This example uses variables and functions to predict properties e.g. proof strength for an austenitic stainless steel at elevated temperatures (20-550° C). The example was created using an expression from Eliasson and Sandström (2000)¹.



This uses the TCFE database. A license is required to run the example.

Example Using the PARROT and EDIT_EXPERIMENT Modules

TCEX36A - USING THE PARROT AND EDIT EXPERIMENTS MODULES

1. "Proof strength values for austenitic stainless steels at elevated temperatures", *Steel Res.*, 71(6–7), 249–254.



The example is divided into parts corresponding to the files in the **tcex36a** folder. It is recommended you open *tcex.36.readme* before continuing with this advanced exercise.

▶ Also see the *Data Optimization User Guide*.

Each problem has "selected" experimental data. The example uses a fictitious binary A-B system where element A is BCC until it melts. Element B is BCC up to 1100 K and FCC above. There is a compound A2B stable in a limited temperature range.

- The creation of the "setup" file is described (*tcex36a.TCM*) where you enter the elements and phases into the Gibbs Energy System (GES) module
- The creation of the experimental data file is described (*tcex 36b.TCM*). When you run the TCEX36a macro, the contents of this macro file is automatically launched and the experimental data file created.
- The actual run in the PARROT module in order to obtain the result (*tcex 36cpd.TCM*)

There are many commands used in this advanced example (listed in alphabetical order):

| | | |
|--------------------------------------------------------|-------------------------------------------------------|-------------------------------------------------------|
| "ADVANCED_OPTIONS" on page 135 | "AMEND_ELEMENT_DATA" on page 204 | "AMEND_PHASE_DESCRIPTION" on page 214 |
| "APPEND_EXPERIMENTAL_DATA" on page 353 | "COMPILE_EXPERIMENTS" on page 261 | |
| "CONTINUE_OPTIMIZATION" on page 262 | "CREATE_NEW_EQUILIBRIUM" on page 159 | "CREATE_NEW_STORE_FILE" on page 263 |
| "DEFINE_COMPONENTS" on page 160 | "EDIT_EXPERIMENTS" on page 263 | "ENTER_PARAMETER" on page 268 |
| "ENTER_PHASE" on page 228 | "LABEL_DATA" on page 300 | "LIST_ALL_VARIABLES" on page 270 |
| "LIST_PHASE_DATA" on page 237 | "LIST_RESULT" on page 272 | "MACRO_FILE_OPEN" on page 114 |
| "OPTIMIZE_VARIABLES" on page 277 | "QUICK_EXPERIMENTAL_PLOT" on page 362 | "READ_WORKSPACES" on page 241 |
| "RESCALE_VARIABLES" on | "SAVE_PARROT | "SAVE_WORKSPACES " on |

| | | |
|--------------------------------------------------|----------------------------------------------------|-------------------------------------------------------|
| page 278 | WORKSPACES" on page 278 | page 305 |
| "SELECT_EQUILIBRIUM" on page 178 | "SET_ALL_START_VALUES" on page 178 | "SET_ALTERNATE_CONDITION" on page 307 |
| "SET_ALTERNATE_MODE" on page 279 | "SET_FIX_VARIABLE" on page 280 | "SET_OPTIMIZING_VARIABLE" on page 282 |
| "SET_STORE_FILE" on page 284 | "SET_WEIGHT" on page 316 | |

Pourbaix Module Examples

TCEX40 - USING THE POURBAIX MODULE

This is the first in a series of examples to demonstrate the advanced POURBAIX module calculations and plotting. This example automatically calculates and plots a Pourbaix diagram for 0.001 m Fe in a 0.1 m NaCl aqueous solution at 25° C and 1 bar. Other diagrams, along with various phase boundaries for the same interactions resulted from the same Pourbaix module calculation, are also plotted.



It is recommended you read the text file *TCEX40-README.txt*, which is located in the **Extended** subfolder.



Also see the *Pourbaix Diagrams Educational Material Guide*.

A so-called Pourbaix diagram is actually a phase diagram with independently-varied acidity (pH) and electropotential (Eh), for a heterogeneous interaction system at a certain bulk composition (that is by default always set as 1 kg of water dissolving a specified amount of metals and other solutes), under a defined temperature and pressure condition.

The PAQ2 Database

The example uses the PAQ2 (TCS Public Aqueous Solution Database using the SIT aqueous solution model) included with your installation. The database contains an AQUEOUS solution phase and REF_ELECTRODE phase (as a reference for electron in aqueous electrolyte systems), as well as some data for various solid phases (solution or stoichiometric) and gaseous mixture phase. The PAQ2 is specially designed for these example calculations of the so-called Pourbaix diagrams (i.e., pH-Eh plots) and other types of phase diagrams or property diagrams in some aqueous-bearing multicomponent heterogeneous interaction systems within the limited chemical framework of Fe-Co-Cr-Ni-C-N-S-H₂O-NaCl, via the Single-Database Option in the advanced POURBAIX module or through the normal TDB-GES-POLY-POST routine.

Additional Examples in this Series

Additional examples (TCEX40A, TCEX40B, TCEX40C, TCEX40D and TCEX40E) are provided to demonstrate options and features in the Pourbaix module and to show more advanced applications of the TCAQ and AQS aqueous solution databases [in the Multiple-Database Option, i.e., with appended data from the SSOL and SSUB databases]. See ["Pourbaix Module Examples TCEX40A to 40E" on the next page](#).

TCEX53 - POURBAIX DIAGRAM CALCULATIONS FOR A HETEROGENEOUS INTERACTION SYSTEM

▶ Also see the *Pourbaix Diagrams Educational Material Guide*.

This example uses the PAQ2 database to calculate some Pourbaix diagrams. The DATABASE_RETRIEVAL (TDB), GIBBS_ENERGY_SYSTEM (GES), POLY3, and POST modules are used for the Fe-X-H₂O-NaCl heterogeneous interaction system, where X = Cr-Ni-Co.



The initial bulk composition of Fe-based alloy in this calculation is just preliminarily assigned, in which the BCC_A2 and/or FCC_A1 solution phase(s) are considered as of primarily interest. For practical calculations, one shall have more precise inputs for the initial bulk compositions of alloys.

Step 1: Single-Point Calculations for H₂O-NaCl system

To demonstrate how to define the molality of NaCl in an aqueous-bearing heterogeneous interaction system.

Step 2: Single-Point Calculations for Fe-X (X = Cr-Ni-Co) system

To demonstrate how to define the initial amount of alloy in an aqueous-bearing heterogeneous interaction system. In this example, we are interested in only the BCC_A2 and FCC_A1 phases in the Fe-based alloy.

Step 3: Single-Point Calculations for Fe-Cr-Ni-Co + H₂O-NaCl system

Step 4: Pourbaix Diagram Mapping for Fe-Cr-Ni-Co + H₂O-NaCl system - define the variables

From the same mapping calculations you arrive at by the end of the example, you can plot more diagrams using a variety of X-Y axis variables.



For a list of pre-defined symbols, go to the end of the tcex53.TCM macro file (open it in a text editor).

Pourbaix Module Examples TCEX40A to 40E

These are the extended examples that are described in ["Pourbaix Module Examples" on page 444](#).

TCEX 40A

This example shows you how to use Option 1 where you **start a completely new**

calculation. It uses a single database. The Pourbaix diagram for 0.001 m Fe in a 0.1 m NaCl solution at 25C and 1 bar is automatically calculated and plotted.



A more advanced version of 40A can be found in TCEX40E, which also uses Option 1 but with multiple databases. However, licenses are required for three types of commercial Thermo-Calc databases.



See "[POURBAIX DIAGRAM Commands for Options 1 to 4](#)" on page 450.

A so-called Pourbaix diagram is actually a phase diagram with independently-varied electropotential (Eh) and acidity (pH), for an heterogeneous interaction system at a certain bulk composition (that is by default always set as 1 kg of water solving a specified amount of metals and other solutes), under defined temperature and pressure conditions. Some property diagrams, along various phase boundaries for the same interactions resulting from the same Pourbaix module calculation, are also plotted, without leaving Option 1.



At the end of this example, a new POLY3 file called *POURBAIX.POLY3* is automatically saved. The following examples (TCEX40B, TCEX40C and TCEX40D) use this same POLY3 file for the calculations. Therefore it is important to make four copies of this file and rename these to TCEX40A.POLY3, TCEX40B.POLY3, TCEX40C.POLY3 and TCEX40D.POLY3. This must be done outside of the Thermo-Calc software and after the TCEX40A calculation and plotting is complete. This is so that the required POLY3 file structure is not lost.



The reason you do not save from within Thermo-Calc is because of how the file is saved. When the command sequence (GO POLY3>SAVE TCEX40A.POLY3>Y) is used, the POLY3 workspace of the POURBAIX calculation results in the POLY3 module monitor and all the initial equilibrium points and the mapping/stepping calculation results are lost as well as parts of the POLY3 file structure (e.g., some definitions of the previously defined POURBAIX-type calculation system).



A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

TCEX 40B

This example shows you how to use Option 2 where you **Open an old (existing) file and plot**

other property diagrams.

Example 40A calculated and plotted the Pourbaix diagram for 0.001 m Fe in a 0.1 m NaCl solution at 25° C and 1 bar. Example 40B reads the original POURBAIX.POLY3 file , and uses the calculated results to plot property diagrams for the same heterogeneous interaction system.



For example 40B, the POLY3 file is not modified. However, it is still recommended that a copy of the original POLY3 file is used so you do not lose the file structure and calculated results.



If you have a POLY3 file generated after choosing Option 4, that file can also be used for Option 2, and vice versa.

TCEX 40C

This example shows you how to use Option 3 where you **Open an old file and make another Pourbaix calculation**. The previously calculated (and copied) POURBAIX.POLY3 file from TCEX40A is edited to make another Pourbaix calculation and plot.

The same chemical system is used (Fe-H₂O-NaCl) but with different P-T-X (pressure-temperature-composition) conditions and without the Gaseous mixture phase. The new conditions are 0.01 m Fe in a 1 m NaCl solution at 200° C and 1 kbar.



In this example, the Gaseous mixture phase for the Pourbaix diagram is not considered.



The POLY3 file is modified and rewritten with the new conditions. As previously recommended, make a copy of the original POLY3 file and rename it (e.g.TCEX40C.POLY3) so you do not lose the file structure and new calculated results.



A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

After the default Pourbaix diagram is generated and refined, you can also use Option 3 to plot property diagrams along different phase boundaries for the same system. These settings are possible from within Option 3 and you do not need to go back to Option 2.

TCEX 40D

This example shows you how to use Option 4 where you **Open an old file and make another stepping calculation**. The previously calculated (and copied) POURBAIX.POLY3 file from TCEX40A is edited to make a stepping calculation and plot.

The same chemical system is used (Fe-H₂O-NaCl) but with different P-T-X (pressure-temperature-composition) conditions and using a POLY3 stepping calculation. The new conditions are 0.01 m Fe in a 0.1 m NaCl solution at 1 kbar and under varied temperature (from 0 to 400° C). The equilibrium conditions are modified and two stepping calculations are done. The same stepping calculation is used to plot property diagrams for the heterogeneous interaction system.

The example also explores settings such as editing the definitions for some system components and their initial bulk composition conditions. This is done through the direct and internal POURBAIX-POLY3 intersection, for a Stepping (or Mapping) calculation inside the Pourbaix module.



The POLY3 file is modified and rewritten with the new conditions. As previously recommended, make a copy of the original POLY3 file (from example TCEX40A) and rename it (e.g. to TCEX40D.POLY3) so you do not lose the file structure and new calculated results.



If you have a POLY3 file generated after choosing Option 2, that file can also be used for Option 4 and vice versa.



A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.

TCEX 40E

This example shows you how to use Option 1 where you **start a completely new calculation**. It uses multiple databases (TCAQ, SSUB and SSOL). The Pourbaix diagram for 0.001 m Fe₉₀Co₅Ni₅ alloy (9E-3 m Fe + 5E-4 m Co + 5E-4 m Ni) in an aqueous solution with 2E-2 m H₂S and 3 m NaCl at 25° C and 1 bar is automatically calculated and plotted.

You need licenses for three Thermo-Calc databases, i.e.

- A: AQS (TGG Aqueous Solution Database; HKF model) or TCAQ (TCS Aqueous Solution Database; SIT model);
- B: SSUB (SGTE Pure Substances Database)

- C: SSOL (SGTE Alloy Solutions Database) or TCFE (TCS Steels/Fe-Alloys Database) or similar.

The TCAQ database contains only an AQUEOUS solution phase (using the SIT model) and REF_ELECTRODE phase (as a reference state for electron in aqueous electrolyte systems). The SSUB database is appended for the Gaseous mixture phase and some pure solid phases (so-called secondary phases formed during aqueous-involving interaction processes), and the SSOL database is appended for various solid solution phases.

The Pourbaix module inside the software also accepts the AQS2 aqueous solution database (using the complete Revised HKF model) in the Multiple Database Option, in addition to the TCAQ2 aqueous solution database (using the SIT model).

POURBAIX_DIAGRAM Commands for Options 1 to 4

Option 1: Start a completely new Pourbaix diagram calculation

Option 1 is used to make a completely new Pourbaix diagram calculation and automatically plot a pH-Eh diagram. i.e., define a new chemical system; specify the T-P-X conditions; calculate the initial equilibria; perform the pH-Eh mapping calculation; plot pH-Eh and various property diagrams.



Many of the commands in Option 1 are also repeated for Options 2 to 4. The details for each command are included with this section unless it is specific to one of the other option choices. The order that the commands display on screen is also different and based on what is entered at the prompts. These prompts are also available in other commands and when applicable a link to that command is included.

```
Consider the GAS phase in calculating a Pourbaix diagram? /Y/
```

You can choose to ignore the GAS mixture phase on a calculated/plotted Pourbaix diagram. However, such a plot is actually not a complete Pourbaix diagram because the thermodynamically-stable phase boundaries between the AQUEOUS solution phase and GAS mixture phase will not be calculated.

- If you enter `y` (the default), GAS mixture phase is always considered.
- If you enter `N` the GAS mixture phase is completely ignored.

```
Use single database? /Y/
```

If you keep the default you are prompted for a database.

```
Combined database: /PAQ2/
```

The default is PAQ2, a database included with all installations.

The following information is provided on screen if you chose Y at the first prompt, Need any instruction on the POURBAIX module? /N/.

DEFINE A CHEMICAL SYSTEM AND ITS INITIAL BULK COMPOSITION

Normally a Pourbaix diagram and its related equilibrium property in a heterogeneous interaction system are calculated under a certain bulk composition, which is usually 1 kg of water with defined amounts of dissolving solute substances. The solutes may either be completely dissolved into the aqueous solution, or be partially dissolved and simultaneously form some solid phases.

Chemical system (elements)

- Default defined elements (solvent H₂O): H and O and specially assigned ZE (electron) and VA(vacancy).
- Prompt specified elements (solutes ELEM): Fe Ni Co Cr C N S Na Cl

Initial bulk composition

- Default defined composition (solvent): 1.0 kg of H₂O
- Prompt specified composition (solutes): x mole of ELEM
- Mass of Water (weight) = 1 kg



When entering solutes in chemical formulas, the first element's letter must be in UPPER case, and second in lower case, for example NaCl, CO₂, CoCl₃, Fe_{0.93}S, NaSO₄-1, and H₂SO₄.

First solute

Enter a solute, e.g. Fe.

Molality of <first solute> [mol/kg] /.001/

Enter a molality for the first solute, e.g. Fe.

Second solute

Enter a second solute and its molality on the same line, e.g. NaCl .1.

Next solute

You can continue to enter solutes. Press <Enter> to skip to the next prompt.

The following information is provided on screen if you chose Y at the first prompt, Need any instruction on the POURBAIX module? /N/.

DEFINED CHEMICAL SYSTEM AND INITIAL BULK COMPOSITION

Solutes have been split up into chemical elements and their mole numbers. If confirmed, the Pourbaix module will, in further steps, count the initial bulk composition in terms of chemical elements.

```
Confirm defined system and initial bulk composition? /Y/
```

If you keep the default (Y) thermodynamic data is retrieved from the database. Then it lists the database's phases for the defined system.

You can then reject or restore phases as required with the next prompts.

```
Reject phase(s) /NONE/
```

```
Restore phase(s): /NONE/
```

Then the program lists the phases retained in the system and you prompted whether this is OK or not.

```
OK? /Y/
```

If you answer Y, then a list of references for the assessed data is displayed on the screen. The next prompt is related to miscibility gap checks, global minimization, saving the information to a POLY3 file, and setting numerical limits.

```
Should any phase have a miscibility gap check? /N/
```

The database usually creates two or more "composition sets" for phases that can have miscibility gaps. However, for some phases this is not done automatically, for example the miscibility gap in the bcc phase in Fe-Cr is usually ignored. But if it is important to include a Cr-rich bcc phase specify this here. It costs some computation time and may make subsequent MAP or STEP processes more difficult to converge. To keep the default (not to have any such phase) press <Enter>. Otherwise answer Y and follow the additional prompts.

```
Enforce Global Minimization Technique in calculations? /N/
```

If you choose Y, the Global Minimization is done when possible (depending on the conditions setting), and a Global Minimization test is performed when an equilibrium is reached. This costs more computer time but the calculations are more robust.

```
Save all functions, variables and tables in POLY3 file? /Y/
```

Choose `y` if you want to save all the defined symbols (functions, variables and tables) into the POURBAIX.POLY3 file, for further normal POLY3 calculations or normal POST post-processing. Choosing yes may result in a large POLY3 file.

Set numerical limits? /N/

▶ ["SET_NUMERICAL_LIMITS" on page 184](#)

The Pourbaix module has a default setting for numerical limits.

- Maximum number of iterations: 20000
- Required accuracy: 1E-6
- Smallest fraction: 1E-15
- Approximate driving force for metastable phases: Y

If you kept the defaults for the above prompts, the program lists the default and pre-defined calculation conditions and you are prompted to confirm.

Confirm defined conditions? /Y/

Now Thermo-Calc calculates the start points. This can take a few moments. Near the end of the calculation there is a list of the default axis variables. The maximum pH limit is calculated precisely and determined automatically by the Pourbaix module as a function of the temperature-pressure conditions and initial bulk compositions of the current defined interaction system. You are prompted to accept these settings.

Accept the default settings for two mapping variables? /Y/

The program now lists the initial equilibria for mapping and continues to calculate the mapping. Then it sets the automatic diagram axes and starts to plot the diagram. But first there are several prompts to guide you.

Any missing phase boundary you could possibly think of? /N/

Sometimes the Pourbaix module may miss some phase boundaries during the mapping process. If you answer `y` you can add additional starting point(s) into the calculation. You are now prompted to specify a pH-Eh coordinate pair, for instance (4.0, -0.15), which is close to the expected phase boundary. However, such additional pH-Eh point should not outside the AQUEOUS/GAS(O₂) or AQUEOUS/GAS(H₂) boundaries; otherwise, the module will fail in finding any new starting point.

The next set of prompts relate to plotting.

Change the pH/Eh steps for smoother curves? /N/

You can modify the mapping steps of X/Y axes for smoother curves; sometimes it may help finding missing phase boundaries by decreasing the pH and Eh increments.

Zoom in? /N/

Change the scaling status for both X and Y axes. The program then asks for minimum and maximum values for the axes. In some cases values are suggested.

Change Curve-Label Option for the diagram? /N/

Change the Curve-Label option to one of the following:

- A: List stable phases along phase boundaries
- B: As A, but curves with same fix phase have same number
- C: List axis quantities
- D: As C, but curves with same quantities have same number
- E: As B, but curves with changing colours
- F: As D, but curves with changing colours
- N: No labels

Usually, Option E or B is good for phase diagrams such as pH-Eh plots, and F or D is good for property diagrams like pH-RC(Fe+2).

► ["SET_LABEL_CURVE_OPTION" on page 369](#)

Add Label-Texts onto the Pourbaix diagram? /N/

Add label text to an area in the diagram. The label is written starting from the specified coordinates. Optionally, let the program automatically add the text by calculating an equilibrium at some specific coordinates and also make a label as the stable phase names in the area. However, such an automatic calculation may fail, especially for a Pourbaix diagram where either pH or Eh is not an intensive variables.

In most cases, the program is able to write the label if the coordinates and texts are specified.

Change the Subtitle of the diagram? /N/

This is the same as the POST module command "[SET_CORNER_TEXT" on page 365](#) → UPPER_RIGHT <SUBTITLE>. The default subtitle is automatically assigned by the POURBAIX module and is based on the defined conditions in the system (temperature, pressure and initial bulk compositions).

If you choose Y then the existing subtitle is displayed and you are prompted to enter a new subtitle or to have None.

New Subtitle /NONE/

You can change the subtitle for all the diagrams in the same POURBAIX run (i.e., within the same Option). The new subtitle that can be altered later at the same option, when further modifying the present graph or when refining any sequentially defined plot. By entering text (empty space at any position is allowed), the new subtitle is defined. By typing OLD, the existing subtitle is kept.

By pressing <Enter> (i.e., accepting None), the subtitle is deleted from all sequential plots, which can be set back later at the same option, too.

Change Axis-Texts? /N/

Change the axis text for both X and Y axes.

Further Refine the diagram in POST Module? /N/

With this option, you can further change the appearance the plot and use any command in the normal POST Module.

► ["POST Module Commands" on page 350](#)

Hard copy of the diagram? /N/

RECOMMENDED RESPONSES

- Hard copy of the diagram? /N/: Y
- CURRENT DEVICE: MS-Windows
- GRAPHIC DEVICE NUMBER /1/: 5
- NEW DEVICE: Postscript portrait mode
- USE POSTSCRIPT FONTS /YES/: Y
- SELECT FONTNUMBER /9/: 27
- NEW FONT: Times-Bold
- FONT SIZE /.35833/: .32
- PLOTFILE : /defaultname/: yourfilename

Save X-Y coordinates of curve on text file? /N/

Write all the current graphic information (generated and modified in the above procedure) on a text file using the DATAPLOT format (see the *DATAPLOT User Guide* or search the online help). This also makes it possible to merge two or more diagrams from separate but similar calculations, or put some experimental data points onto a calculated diagram. You do this by first writing them onto text files with this option and then edit them together (using a general text editor). The program asks for a file name. Accept the default (usually POURBAIX) or use another name. If an extension is not given, the written file is given an extension of *.EXP.

Modify the diagram? /N/

Further modify the appearance of the created plot. This brings you back to the above prompts for changing various features.

Any more diagram? /N/

Make many other plots using the same POURBAIX module calculation file.

Option 2: Open an existing file and plot other property diagrams

COPY AND RENAME THE POLY3 FILE

At the end of a Pourbaix module calculation, a new POLY3 file is automatically saved.



A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.



If you are using a POLY3 file more than once (as is done in the extended examples), it is recommended that you copy and rename the previously-generated POLY3 file. This is so that the required POLY3 file structure and Pourbaix results are not lost. Do this outside of Thermo-Calc i.e. do not save from within Thermo-Calc.



The reason you do not save from within Thermo-Calc is because of how the file is saved. When the command sequence (GO POLY3>SAVE <FILE NAME>.POLY3>Y) is used, the POLY3 workspace of the POURBAIX calculation results in the POLY3 module monitor and all the initial equilibrium points and the mapping/stepping calculation results are lost as well as parts of the POLY3 file structure (e.g., some definitions of the previously defined POURBAIX-type calculation system).

Open an existing POLY3 file created by the Pourbaix module (from a previous Pourbaix calculation Option 1 or 3 or a previous Stepping calculation Option 4), and selectively plotting other property diagrams. i.e., open the old GES and POLY3 workspaces; plot pH-Eh or various property diagrams.

File name /ABCDEF/

The name of a previously saved POLY3 file where the POLY3 and GES5 workspaces is to be read must be specified. You do not need to enter the file extension if it is the default .POLY3 name. The default file name (e.g. ABCDEF) is the most recent specified POLY3-file name or RESULT if there is no workspace already saved in the run. You can press <Enter> or type a specific file name to read the POLY3 and GES5 workspaces from the file.

For Windows, and at the prompt, an **Open file** window displays if a file name is not given or the file path is incorrect. The file type (i.e. POLY3) cannot be changed. Click **Open** or **Cancel** to continue with the selected file.

When the file opens, it confirms on screen what kind of calculation is contained in the POLY3 file. For example: *The loaded POLY3 file is of POURBAIX-MAPPING Calculation.*

On screen it also lists the system components and the default and predefined calculation conditions to enable you to review these.

Next you are given a set of properties that are available to be selected as axis variables for making other diagrams from the same calculation.

| Abbreviation | Definition |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------|
| pH | Acidity |
| Eh | Electronic potential (V) |
| Ah | Electronic affinity (kJ) |
| pe | Electronic activity [$\log_{10} \text{ACRe}$] |
| IS | Ionic strength |
| TM | Total concentration |
| Aw | Activity of water |
| Oc | Osmotic coefficient |
| MF (AQsp) | Mole fractions of aqueous species |
| ML (AQsp) | Molalities of aqueous species |
| AI (AQsp) | Activities of aqueous species |
| RC (AQsp) | Activity coefficients of Aq species |
| Where AQsp is the name of a specific aqueous species, and "*" can be used as a wild sign for all AQSp. It is not necessary to give a complete aqueous species name. However, the entered AQsp name must be unique. If neither AQsp nor * is given, all species are searched. | |



The rest of the prompts are the same as with [Option 1](#) and relate to plotting. Enter ? at any prompt for details.

Option 3: Open an existing file and make another Pourbaix calculation

COPY AND RENAME THE POLY3 FILE

At the end of a Pourbaix module calculation, a new POLY3 file is automatically saved.



A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.



If you are using a POLY3 file more than once (as is done in the extended examples), it is recommended that you copy and rename the previously-generated POLY3 file. This is so that the required POLY3 file structure and Pourbaix results are not lost. Do this outside of Thermo-Calc i.e. do not save from within Thermo-Calc.



The reason you do not save from within Thermo-Calc is because of how the file is saved. When the command sequence (GO POLY3>SAVE <FILE NAME>.POLY3>Y) is used, the POLY3 workspace of the POURBAIX calculation results in the POLY3 module monitor and all the initial equilibrium points and the mapping/stepping calculation results are lost as well as parts of the POLY3 file structure (e.g., some definitions of the previously defined POURBAIX-type calculation system).

Open an existing POLY3 file created by the Pourbaix module and make another Pourbaix diagram calculation i.e. open the old GES and POLY3 workspaces, adopt the defined chemical system, modify the T-P-X conditions, calculate the initial equilibria, perform the pH-Eh mapping calculation and plot pH-Eh or other property diagrams.



The rest of the prompts are the same as with [Option 1](#) or [Option 2](#). Enter ? at any prompt for details.

```
Modify Label-Texts on the Pourbaix diagram? /N/
```

Once some labels are written by the Add-Label-Text command onto the diagram, you can also modify the labels (changing their positions and text contents). The text-size cannot be changed. The program asks which label and you enter its new X/Y coordinates with the new text. The new text must not be longer than the old one.

```
Modify Label-Curve-Option on the Pourbaix diagram? /N/
```

Because some phase-region labels have been written onto the diagram, the Label-Curve-Option might need to be modified, normally to the Option N.

IMPORTANT INFORMATION ABOUT OPTION 3

The default definitions of the Eh and pH quantities in the advanced Pourbaix module (and in the ordinary TDB-GES-POLY calculation routines) should ALWAYS be as below:

$$\begin{aligned} \text{Eh} &= \text{MUR}(\text{ZE}) / \text{RNF} \\ \text{pH} &= -\log_{10} [\text{AI}(\text{H}+1, \text{AQUEOUS})] \\ &= -\log_{10} [\text{ACR}(\text{H}+1, \text{AQUEOUS}) * \text{AH}_2\text{O}] \end{aligned}$$

where RNF is the Faraday constant (96485.309 C/mol), and AH₂O is the molecular weight of H₂O (55.508435 g). MUR(ZE) is the electrochemical potential (ECP; in the unit of J/mol; w.r.t. the standard hydrogen electrode). ACR(H+1,AQUEOUS) is the site-fraction-based activity of the H+1 aqueous species in AQUEOUS solution phase, but AI(H+1,AQUEOUS) [that equals ACR(H+1,AQUEOUS)*AH₂O] is the molality-based activity of the H+1 aqueous species that should be used for defining the pH quantity.

Within an aqueous-bearing heterogeneous interaction system, the fundamental system-components must be H₂O, H+1 and ZE, which are corresponding to the basic elements O & H and the hypothetical electron (ZE) in the aqueous solution phase. For the additional chemical elements in the system, their corresponding system-components shall be defined as in their element forms (such as Fe, Cr, Mn, Ni, Na, Cl, S) or (for some) in their molecular forms (e.g., NaCl, H₂S). The reference state for the H₂O component must always be defined as the solvent species H₂O in the AQUEOUS solution phase under the current temperature (*) and 100000 Pascal (i.e., 1 bar). The reference states for the H+1 and ZE components are by default set as their SER.

Various conventional properties of aqueous solute species I are converted in the following manners:

$$\begin{aligned} \text{ML} &= \text{Y}(\text{AQUEOUS}, \text{I}) * \text{AH}_2\text{O} / \text{YH}_2\text{O} \\ \text{RC} &= \text{ACR}(\text{I}, \text{AQUEOUS}) * \text{YH}_2\text{O} / \text{Y}(\text{AQUEOUS}, \text{I}) \\ \text{AI} &= \text{RC} * \text{ML} \\ &= \text{ACR}(\text{I}, \text{AQUEOUS}) * \text{AH}_2\text{O} \end{aligned}$$

where YH₂O [i.e., Y(AQUEOUS,H₂O)] and Y(AQUEOUS,I) are the site-fractions of solvent H₂O and solute species I.

LIST THE DEFINED AXIS-VARIABLES:

Axis No 1: LNACR(H+1)Min: -34.532525Max: 2.3025851 Inc: 0.8
Axis No 2: MUR(ZE) Min: -150000 Max: 200000 Inc: 7718.85



The default settings (listed above) for two mapping variables [in terms of lnACR(H+1) and MUR(ZE), and their minimum/maximum values and increment steps] are covering the following pH-Eh ranges/steps:

pH: 0.00 -> 14.00, at a step of 0.35
Eh: -1.55 -> 2.07, at a step of 0.08 (V)

The maximum pH limit has been calculated precisely and determined automatically by the Pourbaix module, as a function of the temperature-pressure conditions and initial bulk compositions of the current defined interaction system.

Option 4: Open an Existing file and make another Stepping calculation

Open an existing POLY3 file created by POURBAIX Module (from a previous POURBAIX calculation Option 1 or 3 or a previous STEPPING calculation Option 4), and make a normal STEPPING calculation. i.e., open the old GES and POLY3 workspaces; adopt the defined chemical system; specify one of the T-P-X conditions as the stepping variable; calculate the initial equilibria; perform the stepping calculation; plot various property diagrams.



Many prompts are the same as with [Option 1](#) or [Option 2](#). Enter ? at any prompt for details.

COPY AND RENAME THE POLY3 FILE

At the end of a Pourbaix module calculation, a new POLY3 file is automatically saved.



A reminder that Linux and Mac are case sensitive; when applicable ensure you enter file extensions with capital letters.



If you are using a POLY3 file more than once (as is done in the extended examples), it is recommended that you copy and rename the previously-generated POLY3 file. This is so that the required POLY3 file structure and Pourbaix results are not lost. Do this outside of Thermo-Calc i.e. do not save from within Thermo-Calc.



The reason you do not save from within Thermo-Calc is because of how the file is saved. When the command sequence (GO POLY3>SAVE <FILE NAME>.POLY3>Y) is used, the POLY3 workspace of the POURBAIX calculation results in the POLY3 module monitor and all the initial equilibrium points and the mapping/stepping calculation results are lost as well as parts of the POLY3 file structure (e.g., some definitions of the previously defined POURBAIX-type calculation system).



The stepping calculation modifies the POLY3 file but this can be used for other Stepping calculations inside the Pourbaix module (e.g. repeating Option 4) or in normal POLY3 module.

STEPPING PARAMETERS

The following parameters are suitable for a STEPPING calculation for the defined aqueous-bearing system. Choose one of them as the stepping variable:

```
T Temperature (C)
P Pressure (bar)
pH Acidity
Eh Electronic Potential (V)
N(Comp) Mole of One Component
```

where "Comp" is the name of a specific component as listed below. One should not use any key component (H₂O or H⁺ or ZE) as such a stepping variable, because of that their compositional definitions and variations are determined by the AQUEOUS solution phase in the POURBAIX Module.

An interacting component defined as an element (such as Fe or Na or Cl) can be selected as a stepping variable.

However, if you want to make a stepping calculation with a non-element chemical formula (such as NaCl or CaS₂) as the stepping variable, one must have made some necessary modifications in the POLY3 Module, before reaching this point, by conducting some POLY3 commands as given below (as an example for the system Fe-Na-Cl-H-O):

```
POLY_3: def-component H2O H+1 ZE Fe NaCl Cl
POLY_3: set-ref-state H2O AQUEOUS * 1E5
POLY_3: set-ref-state ZE REF_ELEC * 1E5
POLY_3: change-status phase REF-ELEC=SUSPEND
POLY_3: set-cond b(H2O)=1000 n(H+1)=0 n(ZE)=0
POLY_3: set-cond P=1E5 T=298.15**
POLY_3: set-cond n(Fe)=1E-3 n(Cl)=0 n(NaCl)=3 **
```

** Here the P-T-n(Fe) conditions can be set as what you wanted, while the initial n(NaCl) value must be set as between its minimum and maximum values that you are interested in. Later on, it will be prompted for specifying the n(NaCl) Min-Max-Step values of the stepping calculation.

Stepping variable: /T/

The chosen stepping variable must be one of the suitable parameters listed above.

```
Minimum temperature (C) /15/
Maximum temperature (C) /35/
Increment in temperature (C) /1/
```

The AQUEOUS solution phase under the defined bulk composition and pressure condition is stable only between 0 and 99° C. However, you can make a stepping calculation outside this temperature range, where the AQUEOUS solution phase become metastable. In this case, the resulting POLY3 file is possibly able to be opened by any other option within the Pourbaix module.

Example Using the Tabulate Reaction (TAB) Module

TCEX12 - TABULATION OF THERMODYNAMIC DATA FOR REACTIONS

This example shows a number of independent cases using the TABULATE_REACTION (TAB) module to tabulate thermodynamic data for reactions.



This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- ["TABULATE_REACTION" on page 333](#)
- ["DEFINE_SPECIES" on page 124](#)
- ["ENTER_FUNCTION" on page 222](#)
- ["QUICK_EXPERIMENTAL_PLOT" on page 362](#)
- ["SET_SCALING_STATUS" on page 374](#)
- ["LIST_SUBSTANCES" on page 324](#)
- ["TABULATE_SUBSTANCE" on page 336](#)

Example Using the Reactor Module

TCEX24 - SIMULATION OF THE SILICON ARC FURNACE USING THE REACTOR MODULE

This is a simple reactor model with output of gases at the top and output of condensed phases at the bottom. The gas phase from one segment flows to higher segments, 80% reacts in the first above, 15% in the second above and 5% in the third above.

The condensed phases flow downwards and all of it goes to the next lowest segment. Heat can be added at any module. The only way to specify the initial state of the reactants added to the reactor is to specify the heat content.



This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- ["DEFINE_SPECIES" on page 124](#)
- ["CREATE_STAGE_BOXES" on page 344](#)
- ["CREATE_DIVIDERS" on page 343](#)
- ["CREATE_PIPES" on page 343](#)
- ["START_SIMULATION" on page 347](#)

Application Examples

TCEX09 - CALCULATING A DEW POINT WITH THE POLY3 MODULE

This is an example calculating the dew point in the POLY3 module. The SUBDEMO database is used and included with your installation.

The STEP_WITH_OPTIONS and MAP commands are of note and used in this example.

TCEX10 - PREVENTING Cr₂O₃ CLOGGING IN A CONTINUOUS CASTING PROCESS

The example calculates an equilibrium with suspended or dormant phases and shows how to avoid Cr₂O₃ clogging in a continuous casting process.



This uses the SLAG database. A license is required to run the example.

The origin of this example is that a manufacturer wanted to increase the Cr content of a material from 18 to 25 weight percent but the continuous casting of this material was problematic because solid Cr₂O₃ was formed.

Using Thermo-Calc to calculate the equilibria in the steel/slag system, a simple correction was found: modify the Mn or Si content to decrease the oxygen potential. In Thermo-Calc, you can FIX a phase with zero amount to simulate how to avoid forming this phase. You then release one of the conditions, usually one of the compositions, and this composition is determined by the equilibrium calculation.

These commands are used:

| | | |
|---------------------------------------------|-------------------------------------------------------|-------------------------------------------|
| "DEFINE_SYSTEM" on page 125 | "AMEND_PHASE_DESCRIPTION" on page 214 | "GET_DATA" on page 126 |
| "SET_CONDITION" on page 181 | "LIST_CONDITIONS" on page 170 | "LIST_STATUS" on page 172 |

| | | |
|------------------------------------------------|---------------------------------------------------|----------------------------------------------------|
| "CHANGE_STATUS" on page 152 | "COMPUTE_EQUILIBRIUM" on page 156 | "SET_NUMERICAL_LIMITS" on page 184 |
| "LIST_EQUILIBRIUM" on page 171 | "SET_REFERENCE_STATE" on page 185 | "SHOW_VALUE" on page 188 |

TCEX11 - OXIDATION OF Cu_2S WITH AN $\text{H}_2\text{O}/\text{O}_2$ GAS MIXTURE

This example demonstrates the oxidation of Cu_2S with an $\text{H}_2\text{O}/\text{O}_2$ gas mixture. Thermo-Calc is used to find the optimum O/H ratio (i.e. oxygen potential) as certain oxygen potential values can desulphurize Cu_2S without forming copper oxides.

In Thermo-Calc, the problem reduces to perform equilibria calculations in a Cu-S-H-O system. The amounts of the components should be kept to correct ratio corresponding to Cu_2S and H_2O using a command SET_INPUT_AMOUNTS in POLY3. Initially, O/H = 0.5 is given. Optimum O/H ratio is calculated with the desired calculation conditions. For example, to simulate one phase disappearing, you can FIX the phase with zero amount.

The *tcex11.TDB* file is used to access data and this is included with your installation.

These commands are of also of note and used in this example:

- ["SET_NUMERICAL_LIMITS" on page 184](#)
- ["SET_REFERENCE_STATE" on page 185](#)
- ["SHOW_VALUE" on page 188](#)

TCEX20 - ADIABATIC DECOMPRESSION IN A GEOLOGICAL SYSTEM

This example calculates the adiabatic decompression in a geological system using the geochemical database. The database is included with the file named PGEO.TDB, which is in the same folder as this example.

These commands are of note and used in this example:

- ["DEFINE_SYSTEM" on page 125](#)
- ["DEFINE_COMPONENTS" on page 160](#)
- ["SET_INPUT_AMOUNTS" on page 183](#)
- ["LIST_CONDITIONS" on page 170](#)
- ["SET_CONDITION" on page 181](#)
- ["SHOW_VALUE" on page 188](#)

TCEX24 - SIMULATION OF THE SILICON ARC FURNACE USING THE REACTOR MODULE

This is a simple reactor model with output of gases at the top and output of condensed phases at the bottom. The gas phase from one segment flows to higher segments, 80% reacts in the first above, 15% in the second above and 5% in the third above.

The condensed phases flow downwards and all of it goes to the next lowest segment. Heat can be added at any module. The only way to specify the initial state of the reactants added to the reactor is to specify the heat content.



This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- ["DEFINE_SPECIES" on page 124](#)
- ["CREATE_STAGE_BOXES" on page 344](#)
- ["CREATE_DIVIDERS" on page 343](#)
- ["CREATE_PIPES" on page 343](#)
- ["START_SIMULATION" on page 347](#)

TCEX25 - SIMULATING THE REFINEMENT OF STEEL

This example is based on a typical steel refining process. Raw iron used to produce steel usually has high carbon and silicon content, which is why oxygen is blown into the furnace to burn off carbon. Lime (CaO) is added to form a slag with silica, and the slag can be removed. Alloying elements, such as Mn, Ni, Cr and V are added to produce the desired steel. Since the reaction between O and C increases the temperature, scrap iron is added to keep the temperature constant (it is assumed the furnace is isolated and no heat is lost to the environment).

This example simulates blowing oxygen into a liquid steel of one metric ton (1e6 grams) with 4 w/o C, 2 w/o Si and 1 w/o Mn. 100 moles of CaO (equivalent to 5.6 kg) is added. Keeping the enthalpy constant is the way to simulate the isolation of the furnace. The oxygen reacts with carbon and increases the temperature. After blowing a certain amount of oxygen, scrap iron is added to keep the temperature constant.



This uses the SLAG database. A license is required to run the example.

TCEX27 - CALCULATING CHEMICAL VAPOR DEPOSITIONS (CVD)

This example calculates the chemical vapor deposition (CVD).



This uses the SSUB database. A license is required to run the example.

These commands are of note and used in this example:

- ["DEFINE_COMPONENTS" on page 160](#)
- ["SET_CONDITION" on page 181](#)
- ["ADD_INITIAL_EQUILIBRIUM" on page 133](#)
- ["LIST_AXIS_VARIABLE" on page 170](#)
- ["LIST_INITIAL_EQUILIBRIA" on page 172](#)

TCEX28 - PITTING RESISTANCE EQUIVALENCE (PRE) FOR A DUPLEX STAINLESS STEEL

This example calculates the Pitting Resistance Equivalence (PRE) for a duplex stainless steel.



This uses the TCFE database. A license is required to run the example.

These commands are of note and used in this example:

- ["REJECT" on page 127](#)
- ["RESTORE" on page 128](#)
- ["DEFINE_ELEMENTS" on page 124](#)
- ["AMEND_PHASE_DESCRIPTION" on page 214](#)
- ["EVALUATE_FUNCTIONS" on page 170](#)
- ["SET_START_CONSTITUTION" on page 187](#)

TCEX29 - CALCULATING THE SPECIATION OF A GAS

This example shows how to calculate the speciation of a gas.



This uses the SSUB database. A license is required to run the example.

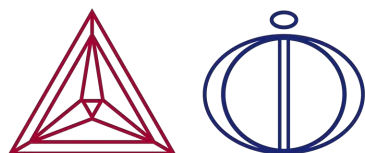
These commands are of note and used in this example:

- ["SET_INPUT_AMOUNTS" on page 183](#)
- ["LIST_CONDITIONS" on page 170](#)

-
- ["SET_CONDITION" on page 181](#)

Data Optimization User Guide

Thermo-Calc Version 2020a



Introduction

In this section:

| | |
|-----------------------------------------|---|
| Introduction to Data Optimization | 3 |
| Data Optimization | 4 |
| The Least-Squares Method | 4 |
| The CALPHAD Approach | 5 |

Introduction to Data Optimization

This guide describes the basic idea behind data optimization, contains brief descriptions of the modules and file types that you work with while doing your optimization, as well as rough outline of overarching workflow that you typically follow when working with optimization.

This guide assumes that you are familiar with using Thermo-Calc Console Mode. It also assumes that you understand the principles of thermodynamics and are familiar with the theoretical foundations of computational thermodynamics.



Press F1 to search the help for information about all the commands available in the Thermo-Calc Console Mode, including PARROT and ED_EXP. Note that the commands listed under PARROT and ED_EXP are only commands that are specific to PARROT and/or ED_EXP. These modules also contain some commands that are also available in POLY.



Thermo-Calc Console Mode [example tcex36](#) is a detailed example of assessment and optimization in Thermo-Calc.

GES5 and GES6 Calculation Engine Version

As of Thermo-Calc version 2019b, the default calculation engine is set to GES6. For PARROT optimization and POURBAIX module users, you need to use GES5. When you try to enter these modules, you are instructed to switch to GES5 using the SET_GES_VERSION command.

▶ ["About the Gibbs Energy System \(GES\) Module" on page 36](#)



To globally set the default from GES6 back to GES5, go to the **Tools → Options** → ["General" on page 37](#) tab and click **Version 5** for the *Preferred Gibbs Energy System* setting. The ["SET_GES_VERSION" on page 118](#) Console Mode command is used to change GES versions for a single Thermo-Calc session.



Contact Thermo-Calc Software AB at info@thermocalc.com for more information about the changes or if you encounter any issues you think are related to the new version of the calculation engine.

Data Optimization

In a thermodynamic database, each phase in a system is characterized using a mathematical model of its Gibbs energy. The Gibbs energy of a phase depends on various state variables. It can be defined individually even in a heterogeneous system with many stable phases since the properties of one phase are completely independent of the properties of the other phases in the system. In most alloy systems, the thermodynamic properties of a phase can be modelled by expressing how the Gibbs energy depends on temperature and composition. State variables such as pressure, volume or entropy can also serve as parameters in the Gibbs energy expression. The Gibbs energy of the whole system is the sum of the products of the Gibbs energy of each phase multiplied by the amount of that phase.

How the Gibbs energy of the phase varies with various state variables is determined by a mathematical model and how various adjustable parameters of the model is set. By optimizing these parameters, you can calculate the thermodynamic properties of a system under various conditions (by calculating phase diagrams for example). The thermodynamic properties themselves are functions of temperature, pressure or composition. They include, among other properties, standard enthalpy of formation, entropy, heat capacity, molar volume, thermal expansivity, compressibility and Curie temperature for magnetic transformations.

Data optimization is about adjusting the model parameters so that calculated equilibria fit well with experimental data. An important part of a data optimization is therefore collecting and assessing available experimental and theoretical information about phase equilibria and thermochemical properties of a system.

When you optimize the parameters of the model of a phase, you put what is called optimizing variables into the Gibbs energy expressions of those parameters. During the optimization, the values of these variables are varied in order to find a fit between the calculated equilibria and the experimental data that you base the optimization on. Once you have settled on a Gibbs energy expression for a certain parameter of a phase of the element, then you must stick to this expression in all future optimizations involving the element. If you do not do this, then you must re-optimize all previous systems that involve this element when the expression is changed.

The Thermo-Calc software allows you to optimize parameters that characterize not only binary systems, but also ternary system and systems of even higher orders. You can even optimize parameters that characterize systems of different orders at the same time.

The Least-Squares Method

Data optimization in Thermo-Calc is based on the least-squares method for fitting values calculated on the basis of a model with observed quantities. The software is accordingly

trying to find the optimizing variable values that lead the minimized sum of the squares of the differences between the calculated values and the observed quantities (that is, of the errors or residuals).

The least-squares method works best under the following conditions:

- The observed quantities have a Gaussian probability distribution.
- The observed quantities are only subject to random errors.
- The different observations (experiments) are uncorrelated
- The standard deviation of each observation can be estimated.
- The number of observations is large.
- The models used give precise predictions.

Of course, these conditions are usually not all met in a normal thermodynamic assessment. But even in non-ideal conditions, there is no known method that works better than the least-squares method.

The CALPHAD Approach

The data optimization functionality in Thermo-Calc works according to the CALPHAD approach to computational thermodynamics. This approach builds on the development of models that accurately represent thermodynamic properties for various phases. These models enable you to predict the thermodynamic properties of multicomponent systems-based data concerning binary and ternary subsystems. The predictions can take many factors into accounts, such as, for example, crystallography, type of bonding, order-disorder transitions and magnetic properties.

CALPHAD is originally an abbreviation of *CAL*culat*ion of PH*ase *Diagrams*, but as the approach has expanded in scope, it now stands for *computer coupling of phase diagrams and thermochemistry*.

REFERENCES

For in-depth information about CALPHAD as well as data optimization, see *Computational Thermodynamics – The Calphad Method* by Hans Leo Lukas, Suzana G. Fries and Bo Sundman (Cambridge University Press, 2007). CALPHAD was given its first general description in *Computer Calculations of Phase Diagrams* by Larry Kaufman and Harold Bernstein (Academic Press, 1970). The book contains some case studies of optimizations using Thermo-Calc.

Information about the concept of 'lattice stability' (which is important for the development of multicomponent thermodynamic databases) can also be found in the paper *Hume-Rothery and Calphad Thermodynamics* by Larry Kaufman, published in *Calphad and Alloy Thermodynamics*, edited by Patrice E.A. Turchi, Antonios Gonis, Robert Shull (The Minerals, Metals & Materials Society, 2002), pp. 3-19.

Working with Data Optimization in Thermo-Calc

In this section:

| | |
|----------------------------------------------|----|
| Data Optimization in Thermo-Calc | 8 |
| Data Optimization Workflow | 8 |
| The PARROT Module | 9 |
| The EDIT_EXPERIMENTS Module | 10 |
| Data Optimization in Other Modules | 10 |
| Optimization File Types | 10 |
| Optimization Workspaces | 11 |
| Method for Optimization and Simulation | 12 |

Data Optimization in Thermo-Calc

The actual performance of the optimization of a system is primarily done in the PARROT module, and in its sub-module ED_EXP. The POLY and POST modules are used to calculate and plot property or phase diagrams based on the optimized variables. This allows you to visually assess how good a fit you have achieved between your calculated results and your experimental data.

The end result of a successful optimization is typically an updated Thermo-Calc database file (with filename extension *.TDB) or a new database file.

Data Optimization Workflow

When you carry out an optimization using Thermo-Calc, you typically follow a workflow as outlined below.

1. Collect experimental data about your system from various sources such as journal articles and reports.
2. Create a POP-file in which you enter the experimental data you have collected.
3. Create a setup macro file in which you define your system and the variables you want to optimize. A useful general procedure is to first find a minimum set of variables that allows you to calculate most of the experiments.
4. Run the setup macro file.
5. Compile your POP-file. This file often contains errors, which need to be corrected, and the file recompiled several times before the compilation is completed without errors.
6. In the ED_EXP module, check that the experiments in your POP-file reach equilibrium with reasonable results. If any experiments do not reach equilibrium with reasonable results, then try changing the starting values on equilibrium conditions (such as composition) to see whether the equilibrium can be computed after all. If this does not work, then you can temporarily exclude the experiment from the optimization. At a later stage in the optimization, when the optimizing variables have different values, you can check whether the experiments can be computed with reasonable results.
7. Back in the PARROT module, run the first optimization cycle and evaluate the feedback in the console. You can also plot diagrams in the POLY module that allow you to visually inspect the fit between calculated optimization results and the experimental data. If you are not satisfied with the fit, then enter the ED_EXP module again and adjust the weights of the experiments in a way that is likely to improve the fit and run another optimization cycle. Reiterate until you are satisfied with the fit.

8. Once you get the optimization stable and smooth with the minimum set of variables chosen in step 3 above, try using different sets of variables to see whether improvements are possible.
9. When you are satisfied with the fit between calculated results and experimental data with your final set of optimizing variables, update your setup file and POP-file. In the setup file, enter the calculated optimizing variable values as the variables' start values. In the POP-file, enter the final weights of the experiments. With these files updated, you can easily regenerate the parameter values of your optimized system. Having the files updated also makes it easier to optimize the system again in light of new data or new theoretical models.
10. Finally, update the database with your calculated results or create a new database with information about the system that you have optimized.

The PARROT Module

The PARROT module consists of a comprehensive subroutine package for data evaluation of thermodynamic model parameters from experimental data. The module has 99 variables that you can use for optimization and the module can handle a thousand experimental measurements in an optimization. However, there are limits on the simultaneous numbers of variables and experiments. These limits are listed at each optimization.



The PARROT module is part of the Thermo-Calc software. The module is not included in the software development kits (SDKs).

The experimental data is entered and edited in a sub-module of PARROT: ["The EDIT EXPERIMENTS Module" on the next page.](#)

GES5 and GES6 Calculation Engine Version

As of Thermo-Calc version 2019b, the default calculation engine is set to GES6. For PARROT optimization and POURBAIX module users, you need to use GES5. When you try to enter these modules, you are instructed to switch to GES5 using the SET_GES_VERSION command.



["About the Gibbs Energy System \(GES\) Module" on page 36](#)



To globally set the default from GES6 back to GES5, go to the **Tools → Options** → ["General" on page 37](#) tab and click **Version 5** for the *Preferred Gibbs Energy System* setting. The ["SET GES VERSION" on page 118](#) Console Mode command is used to change GES versions for a single Thermo-Calc session.



Contact Thermo-Calc Software AB at info@thermocalc.com for more information about the changes or if you encounter any issues you think are related to the new version of the calculation engine.

The EDIT_EXPERIMENTS Module

The EDIT_EXPERIMENTS module, or ED_EXP for short, is used for entering, evaluating and editing experimental data. To enter the module, go to "[The PARROT Module](#)" on the [previous page](#) and then issue the command "[EDIT_EXPERIMENTS](#)" on page 263.

Since ED_EXP uses the POLY module for doing equilibrium calculations of experimental data points, many POLY commands are also available in the ED_EXP module. However, the commands may work somewhat differently in the two modules. There are also unique ED_EXP commands which are not found in POLY.

When you execute ED_EXP commands, the PARROT workspace is modified. However, note that you must always first use "[READ WORKSPACES](#)" on page 241 in ED_EXP before doing anything in the module. The command loads the experimental data that you are going to work with during the optimization. Furthermore, before leaving ED_EXP you must use "[SAVE WORKSPACES](#)" on page 305 or the results of your work in the ED_EXP module is lost.

Data Optimization in Other Modules

All kinds of thermodynamic data, calculated equilibrium states or dynamic parameters are transferred back and forth between the PARROT and the GIBBS module as well between these and the POLY module. Whenever an optimization run is performed, PARROT calls the GIBBS module for stored system definition data and model parameters.


In Thermo-Calc, the GIBBS module (the Gibbs Energy System) handles the models of the various phases that can form in a multicomponent system. It stores thermodynamic data and performs various Gibbs energy equilibrium calculations. It contains subroutines to analytically calculate the first and second partial derivatives of integral Gibbs energy with respect to any set of variables. Many thermodynamic models for various types of substances are implemented in the module. Some commands that are available in the PARROT module are also available in the GIBBS module.

In the GIBBS module, parameters of the Gibbs energy models are referred to as *TP-functions*.

PARROT calls the POLY module for equilibrium calculations. The POLY module is used for calculating and storing complex heterogeneous equilibria.

Optimization File Types

These are the important files you work with when optimizing.

| File type | Description |
|-------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| POP-file | The POP-file (Parrot OPTimization file) is the file that contains all the experimental data that you use for optimizing Gibbs energy values for your system. The POP-file is a plain text file that contains ED_EXP commands. By default, the file has the filename extension *.POP in Thermo-Calc. |
| Setup file | The setup file is a Thermo-Calc macro file (*.TCM). This file typically contains commands that define your system, opens the PARROT workspace (and associated GIBBS and POLY workspaces) and sets optimizing variables. |
| Other macro files | It is often useful to have other macro files than the setup file at hand while you are doing your optimization. For example, it is convenient to have a macro file that automatically plots phase diagrams or other diagrams based on the latest values of your optimizing variables. An optimization process typically involves many optimization cycles, so this operation needs to be done many times during a typical optimization. |
| Workspace files | The PARROT module has its own workspace with dynamic memories, similar to the workspaces of POLY and GIBBS. It is stored and updated in a PARROT workspace file with the filename extension *.PAR. The workspace file is a binary file whose format is hardware dependent. This means that the format is unique for each type of CPU. Hence, a workspace file saved on a computer with one type of CPU cannot be used on a computer with another type of CPU. |
| EXP-file | <p>The EXP-file is a plain text file with information in the form of DATAPLOT Graphical Language commands. These commands can specify some or all of the data points in your POP-file. This allows you to plot these data points on top of your plotted optimization results (with the POST commands "APPEND_EXPERIMENTAL_DATA" on page 353 or "QUICK_EXPERIMENTAL_PLOT" on page 362). You can then visually assess the fit between these results and the experimental data. The PARROT workspace is not influenced in any way by the creation or use of EXP-files.</p> <p> <i>DATAPLOT User Guide</i> included with this documentation set.</p> |

Optimization Workspaces

When writing the setup file, you enter a ["CREATE_NEW_STORE_FILE" on page 263](#) command which creates a PARROT workspace file. Alternatively, select an existing PARROT workspace file with ["SET_STORE_FILE" on page 284](#). The workspace file is automatically updated and saved with the latest optimization results (after each use of the ["OPTIMIZE_VARIABLES" on page 277](#) command). You can also explicitly instruct Thermo-Calc to save the workspace using ["SAVE_PARROT_WORKSPACES" on page 278](#). If you want to get rid of your latest changes and return to the state of your workspace when it was last saved, use ["READ_PARROT_WORKSPACES" on page 277](#).

When the PARROT workspace is saved, parts of the POLY and GIBBS workspaces are also saved to the PARROT workspace file, along with the PARROT workspace itself. Using the POLY command ["SAVE_WORKSPACES" on page 176](#) creates a new POLY3 file, nothing is saved to the PARROT workspace file.

If you do any POLY calculations based on data in the current workspace file, then a *.POLY3 file is created, which contains a copy of the current set of parameters. If you continue on your optimization and read the old *.POLY3 file, then the new set of parameters is overwritten with the old set. It is therefore recommended that you never read a *.POLY3 or *.GES5 file while you are doing an optimization.

Method for Optimization and Simulation

The PARROT module typically uses ordinary POLY minimization for equilibrium calculations. The global minimization technique that is used in POLY cannot be used because it automatically creates new composition sets which corrupt the PARROT workspace. Furthermore, the equilibrium definitions that you use as input for your optimization must each be attributed to a specific phase. Some of these definitions may specify some local or partial equilibrium state rather than a global minimum. However, it is possible to use the global minimization technique for some equilibrium calculations by using the ED_EXP command ["ADVANCED_OPTIONS" on page 135](#) with the `Toggle_Alternate` option.

Optimization in PARROT is performed on the basis of a 'maximum likelihood' principle. According to this principle, the best fit between various calculated results and all the input of experimental data is found where the sum of the square of the weighted residuals is at its minimum.

Typically, the results of an optimization is considered to be better the fewer optimizing variables that are needed to get the same level of fit between computed results and experimental data. If you can get almost the same fit using eight instead of twelve parameters, then this should be considered to be a significant improvement. When more parameters are used, the values of the individual parameters tend to become unrealistic. This is particularly true when it comes to temperature-dependent parameters. However, relatively small differences in the number of parameters are often insignificant. For example, it does not typically matter whether you used 24 or 25 parameters to reach a certain degree of fit.

It is often difficult to compare the quality of different optimizations based on the number of optimizing variables that have been optimized. Since you may rely more or less heavily on different pieces of available experimental data (and do so with good reason), it is possible that two different users could end up with very different numbers of parameters for the same system. For example, suppose you optimize the Fe-Al system to incorporate it into an Al database, while someone else optimizes the same system to incorporate it into an Fe database. In this situation, the two of you would probably make different judgements about which experimental information your calculated results must have a good fit with.

Creating the POP-File

Before starting an optimization in Thermo-Calc, you must collect relevant experimental data about your system that is available in the research literature. This data is then entered in the POP-file. The experimental data points and measurements are entered in this plain text file in the form of ED_EXP commands.

The syntax of the POP-file is in principle independent of the models used for describing the phases in the system.

In this section:

| | |
|-------------------------------------------------|----|
| Experimental Information | 14 |
| POP-File Syntax | 17 |
| Entering Experimental Information | 18 |
| Using Stability Conditions | 25 |
| Grouping Equilibria with Labels | 26 |
| Dividing the POP-File into Several Blocks | 26 |

Experimental Information

An optimization of thermodynamic model parameters should be based on a range of reliable experimental results that is as wide as possible, as well as on empirical or semi-empirical correlations and theoretical considerations. During an optimization in Thermo-Calc, many kinds of thermochemical and thermophysical data can be mixed and used together.

The information needed for an optimization represent measurements of thermodynamic parameters in the system at equilibrium. These can be measurements of any of the thermodynamic quantities that can be set as conditions in Thermo-Calc. The information may represent measurements of activities or enthalpies in single-phase regions for example, or solubilities or transformation temperatures in a multi-phase region.

For each equilibrium that is used in the optimization, at least one quantity must have been measured and you also need to know the conditions that must be set to compute the system's equilibrium state. For example, consider a binary system in a single-phase region. Suppose that you have measured the temperature, pressure, composition and the chemical potential. Three of these quantities are necessary to specify the equilibrium state and the forth can be used as experimental information to model the phase.

If you have a two-phase region and know the temperature and pressure conditions, as well as which the stable phases are, then you could use the compositions of one or both phases as experimental data. The former information about the conditions is sufficient to determine the equilibrium. The experimental information can then be used to optimize the parameters that are used to characterise and model the system.



For examples how to enter various kinds of experimental data in the POP-file, see ["Experiments and Experimental Data" on page 57](#).

CONFLICTING OR MISSING INFORMATION

You are likely to sometimes have inconsistent or conflicting experimental information. In principle, all available experimental data should still be entered into the POP-file, unless you have good reasons to exclude some information. For example, if you have reason to believe that the samples used in some experiments were not pure, then these experiments could be excluded from the POP-file.

For some systems, you have very little experimental data to go on. When this is the case, do not try to fit the available data uncritically with high accuracy without considering possible errors. You can look for data in systems with similar elements to get an idea about what the reasonable estimates of data that is lacking could be. Or you can use calculations from first principles or semi-empirical methods to get reasonable estimates that can be used as experimental data.

INVARIANT EQUILIBRIA INFORMATION

The most valuable experimental information for an optimization is information about stable invariant equilibria. An invariant equilibrium is such that neither pressure, temperature nor composition can be changed without there being a change in the set of phases present in the system. It is recommended that all information about invariant equilibria for a system is included in the POP-file. These equilibria need not all be based on explicit experimental measurements of thermodynamic properties.

Reasonable estimates from available experimental data are often useful to include in the POP-file. Such estimates, which should be based on the available experimental data, helps Thermo-Calc find a good set of start values on the optimization variables. However, at the end of the assessment, these estimated equilibria should be excluded and you should complete the optimization based only on the experimental information that is based on measurements.

With some experience from phase diagram evaluation, it is possible to make reasonable estimates of metastable invariant equilibria. Such estimates helps reduce the number of phases that are assessed simultaneously during the optimization. For example, you may assume that a certain intermediate phase does not form in a system. Then extrapolate the liquidus curves below the stable three-phase equilibria and finally, estimate temperatures and compositions of metastable three-phase equilibria between two other phases and the liquid.

Another useful technique is to extrapolate a liquidus line from a peritectic equilibrium to estimate the congruent melting temperature of a compound. This estimate may be more useful than the information about the peritectic equilibrium itself as the equilibrium involves only two phases.

EQUILIBRIA IN HIGHER-ORDER SYSTEMS INFORMATION

When you optimize a binary system, the available experimental information can often be described equally well by very different sets of parameters. Information about ternary and higher order systems that include the components of the binary system are then often useful for optimizing the binary system (the same is true of information about quaternary system with respect to optimizing ternary systems). Often, it is only when you extrapolate the optimized parameters to a higher-order system that you can judge which of the sets of model parameters that is best. Sometimes information from several ternary systems is required to make a reliable judgement about which set of parameters best describes a particular binary system.

HEAT CAPACITIES INFORMATION

If you want to optimize your system based on data about heat capacities, then the corresponding parameters should first be optimized separately before you perform the general optimization of your system. The parameters should be kept fixed during the general optimization. This is because it is normally not possible to optimize heat capacity data together with other data in a meaningful way. If you do this, then it is very likely that the parameters related to the heat capacity are badly determined.

POP-File Syntax

It is recommended that you specify an experimental equilibrium as close as possible to actual experimental conditions. Ideally, there is information about the set of stable phases, temperature, pressure and some or all compositions for the equilibrium.

In addition, it is recommended that you keep the POP-file well-organised and extensively commented. This is especially important if someone else reassesses the system when new experimental information is available.

If you have too many equilibria defined in your file, or if you define equilibria with different sets of components in the same file, then you must divide the POP-file in *blocks* (using the ["FLUSH_BUFFER" on page 298](#) command). You know whether you have defined too many equilibria for one block when you compile the file. A too large number of equilibria leads to an error message when the file is compiled.

If you use the ["DEFINE_COMPONENTS" on page 160](#) command, then it must be the first command in the POP-file (or if you have several blocks, DEFINE_COMPONENTS can also be put as the first command after FLUSH_BUFFER). This is because the command automatically reinitiates the current workspace, so the effect of any commands placed before it are not saved.



The last command in the POP-file should always be ["SAVE_WORKSPACES" on page 305](#).

LEGAL COMMANDS IN A POP-FILE

The following commands can be used in a POP-file.

- ["ADVANCED_OPTIONS" on page 135](#)
- ["CHANGE_STATUS" on page 152](#)
- ["COMMENT" on page 291](#)
- ["CREATE_NEW_EQUILIBRIUM" on page 159](#)
- ["DEFINE_COMPONENTS" on page 160](#)

-
- ["ENTER_SYMBOL" on page 167](#)
 - ["EVALUATE_FUNCTIONS" on page 170](#)
 - ["EXPERIMENT" on page 296](#)
 - ["EXPORT" on page 298](#)
 - ["FLUSH_BUFFER" on page 298](#)
 - ["IMPORT" on page 299](#)
 - ["LABEL_DATA" on page 300](#)
 - ["SAVE_WORKSPACES" on page 176](#)
 - ["SET_ALL_START_VALUES" on page 178](#)
 - ["SET_ALTERNATE_CONDITION" on page 307](#)
 - ["SET_CONDITION" on page 181](#)
 - ["SET_NUMERICAL_LIMITS" on page 184](#)
 - ["SET_REFERENCE_STATE" on page 185](#)
 - ["SET_START_VALUE" on page 187](#)
 - ["SET_WEIGHT" on page 316](#)
 - ["TABLE_HEAD, TABLE_VALUES and TABLE_END" on page 318](#)

Entering Experimental Information

A POP-file in Thermo-Calc (*.POP) mainly consists of descriptions of equilibria, each equilibrium describing a data point that is based on an experiment from the existing literature on your system. An equilibrium is specified using ED_EXP commands.

The following is an example of a specification of an equilibrium with a single stable phase in the Au-Cu system. Equilibria with a single stable phase are often from experiments where enthalpies of mixing or chemical potentials have been measured.

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE LIQUID=FIX 1
SET_CONDITION T=1379 P=1E5 X(LIQUID,AU)=0.0563
SET_REFERENCE_STATE AU LIQ * 1E5
SET_REFERENCE_STATE CU LIQ * 1E5
EXPERIMENT HMR=-1520:200
COMMENT Measurement by Topor and Kleppa, Met trans 1984
```

Creating a New Equilibrium

The first command in an equilibrium specification is always ["CREATE_NEW_EQUILIBRIUM" on page 159](#). This command takes two integers as arguments. The first integer should specify a unique identifier that can be used later to refer to the equilibrium in question. The second integer is an initialisation code 0, 1 or 2:

- Code 1: This means that all components are entered but all phases are suspended. This code is appropriate in most cases.
- Code 0: This means that all components and phases in the equilibrium are suspended initially. This code is needed if you are using experimental data about systems of different orders simultaneously, such as data about both binary and ternary systems for example.
- Code 2: This means that all components and phases are initially entered.

EXAMPLE

For example, the first command in the example above creates an equilibrium data point with the unique identifier 1. All components of the system are entered but all phases are suspended:

```
CREATE_NEW_EQUILIBRIUM 1 1
```

Setting Equilibrium Conditions and its Uncertainty

All the equilibrium-related commands that are placed in between two ["CREATE_NEW_EQUILIBRIUM" on page 159](#) commands are interpreted as specifying the conditions of the equilibrium created by the first command. The values of these conditions should be based on the conditions specified in the experiment that you base the equilibrium definition on.

EXAMPLE

In the example, the ["CHANGE_STATUS" on page 220](#) command specifies that the equilibrium is a single-phase equilibrium with the liquid phase.

```
CHANGE_STATUS PHASE LIQUID=FIX 1
```

Furthermore, the temperature is 1379 K, the pressure is 1 bar (1E5 Pa) and the mole fraction of Au is 0.0563.

```
SET_CONDITION T=1379 P=1E5 X(LIQUID,AU)=0.0563
```

Sometimes you have reason to think that some information about an equilibrium condition may not be accurate. If this is the case, then you specify the degree of uncertainty for a condition with a colon after the condition quantity, directly followed by either an absolute value or a percentage. For example, if you have reason to doubt the reliability of the Au mole fraction measurement, then you could write:

```
SET_CONDITION T=1379 P=1E5 X(LIQUID,AU)=0.0563:10%
```

This indicates that you think the Au mole fraction is between 0.0507 and 0.0619. PARROT calculates the equilibrium twice, once for 0.0507 and once for 0.0619, and then computes the change of each experimental value between these two equilibria. This change is used to modify the uncertainty specified for the experimental value.

► ["Entering the Experimental Value and its Uncertainty" on the next page](#)

The possibility of specifying uncertainties on conditions may be useful when you have experimental data about a ternary system. In a binary system, a tie-line is determined by the two phases, the temperature and the pressure. Measurements of the compositions of both phases can then be used as experimental data. To specify the tie-line in a ternary two-phase equilibrium one of the four compositions must also be set as a condition. If the measurement of this composition has the same uncertainty as the other compositions, then you can assign this same degree of uncertainty both to the composition selected as a condition and the compositions selected as experimental data. Alternatively, the sample (overall) composition could be used as a condition and all four phase compositions could be used as experiment values. These phases must have the status *entered* (not fixed) since the relative amount of each is unknown.

Setting Reference States

If you want to specify a non-default reference state for one or several of your system components, then you do this with the ["SET_REFERENCE_STATE" on page 185](#) command. In the following example, the reference state for the liquid phase is set to current temperature (*) and a pressure of 1E5 Pa.

EXAMPLE

```
SET_REFERENCE_STATE AU LIQ * 1E5  
SET_REFERENCE_STATE CU LIQ * 1E5
```

Note that in order for these reference states to be taken into account when the measurement of the enthalpy per mole of the system is entered with experiment, the R-suffix must be used.

Entering the Experimental Value and its Uncertainty

The "[EXPERIMENT](#)" on [page 296](#) command is used to specify the quantity that the calculated results should be fitted to. When specifying this quantity, you both specify the measured quantity itself and your estimation of the uncertainty of this value.

EXAMPLE

In the example, the EXPERIMENT command specifies the enthalpy per mole of the system, where this value is specified with respect to non-default reference states that you have set in the equilibrium specification:

```
EXPERIMENT HMR=-1520:200
```

The value before the colon is the quantity of the variable. The value after the colon is an assessment of the uncertainty of this quantity. A higher value means a greater uncertainty. In the example, the uncertainty has been specified with an absolute value but it could also be specified in percent of the quantity:

```
EXPERIMENT HMR=-1520:13%
```

Several experiments can be specified after the experiment command. Besides assigning values to conditions, it is also possible to specify that a certain quantity is greater than or less than a certain value. For instance, the following command would specify that the activity of the C-component is less than 0.01 and the mass fraction of the BCC phase of Ag is greater than 0.05:

```
EXPERIMENT ACR(C)<0.01:0.001 W(BCC,AG)>0.05:10%
```

Note that an experimental quantity can typically also be treated as an equilibrium condition, and vice versa. Which measured quantities that you treat as conditions and which quantities you treat as experimental data should be based on the accuracy of the different measurements. In most cases, the quantity that is based on the experimental technique with the lowest accuracy should be used as the experimental value.

Entering Many Equilibria as a Table

When one thermodynamic variable (e.g. heat capacity) has been measured as a function of another (e.g. temperature), then experimental data is often presented as a table. By using the TABLE_HEAD, TABLE_VALUES and TABLE_END commands, you can enter such experimental information into the POP-file in the form of a table. These three commands should always be used together and must be entered in the right order. See ["TABLE_HEAD, TABLE_VALUES and TABLE_END" on page 318](#).

The TABLE_HEAD command is followed by a number. This number identifies the table as a whole, but also uniquely identifies the first equilibrium that is included in the table. This numeric identifier is incremented by one for each additional equilibrium in the table. Each row in the table represents one equilibrium. Thus, the equilibrium defined by the first row in the table above (on the line immediately below TABLE_VALUE) is uniquely identified with the number 1, the equilibrium defined by the second row by number 2, and so on until the last equilibrium on the sixth row, which is identified by the number 6.

Since the unique identifiers of the equilibria in the table are automatically generated from the unique numerical identifier that you give to the table, the unique numerical identifier that is normally given to the ["CREATE_NEW_EQUILIBRIUM" on page 159](#) command is replaced by two at signs (@@).

At least one of the equilibria conditions specified with the ["SET_CONDITION" on page 181](#) command must be a condition whose value is set by the numbers in one of the table columns. To assign the numbers in a column to a condition, use the syntax `SET_CONDITION <condition>=@<column number>`. For instance, in the example above, the mole fraction of $X(\text{AlO}_3/2)$ is for each equilibrium given by the number in the first column of the table.

At least one of the measured variables that are entered with the experiment command must be a variable whose value is set by the numbers in a table column. To assign the numbers in a column to a measured variable, use the syntax `EXPERIMENT <variable>=@<column number>`. In the example above, the measured temperature for each equilibrium is given by the number in the second table column.

The actual table should be entered between `TABLE_VALUES` and `TABLE_END`. Separate the columns with tabs or any number of spaces. The columns do not have to contain numbers, but can also contain other types of values, such as phase names for example. If a column contains text with spaces or special characters, then the text must be surrounded by double quotes ("ABC DEF&ghi", for example). The table may have columns that are not used, but each row must have exactly the same number of columns.

EXAMPLE

The following block of commands exemplifies how a table can be entered into a POP-file:

```
TABLE_HEAD 1
CREATE_NEW_EQUILIBRIUM @@ 1
CHANGE_STATUS PHASE TETR=FIX 0
CHANGE_STATUS PHASE ION=ENT 1
SET_CONDITION P=101325 N=1 ACR(O2,GAS)=.21 X(ALO3/2)=@1
EXPERIMENT T=@2:5
TABLE_VALUE
0.46082476
0.57142380
0.66822276
0.7496 2176
0.50382426
```

0.63132249

TABLE_END

Setting Site Fraction Start Values

In some systems, you have to set non-default composition start values on some experiments in order to get them to converge properly during optimization. This may be important if your system has a miscibility gap for example, in which case several equilibria with different compositions exist at certain temperatures. In such cases, you have to make sure it is specified in the POP-file which side of the miscibility gap the equilibrium is on. The calculated equilibrium could otherwise end up on the wrong side, resulting in a large error.

In the POP-file, you can set the site fraction of a constituent on an equilibrium with ["SET_START_VALUE" on page 187](#).

EXAMPLE

For example, the following command sets the composition start value of VA constituent of the FCC_A1 phase to 0.99:

```
SET_START_VALUE Y (FCC_A1,VA#2)=0.99
```

Setting the mole fraction for a component in a phase is not as reliable as setting the site fraction.

Additional equilibria entered after the last SET_START_VALUE command are automatically given a similar start value if the following command appears previously in the POP-file:

```
SET_ALL_START_VALUES Y
```

If start values are not set automatically for phase constituents, then you may have to set the composition start value for each equilibrium (or table of equilibria) separately.

Commenting About an Equilibrium

The COMMENT command inserts a comment about the equilibrium that is saved to the PARROT workspace file when the POP-file is compiled. The comment must be entered on one line.

Comments can also be entered immediately after a dollar sign (\$), but these are not saved to the PARROT workspace. Instead, these comments are ignored by Thermo-Calc when the POP-file is compiled.

Simultaneous Use of Binary and Ternary Experiments

You can use experimental information about binary and ternary systems (as well as systems of even higher order) in the same POP-file and optimization. To do this, you must inform the PARROT module that not all components of the ternary system (or system of even higher order) should be considered. This allows you, for example, to use experimental information about a binary equilibrium that exists within a ternary system.

Use ["CHANGE_STATUS" on page 220](#) with the keyword component and which components that should be entered. You should also give the initialization code 0 (rather than 1) to the ["CREATE_NEW_EQUILIBRIUM" on page 159](#) command. This code indicates that all components must be entered.

EXAMPLE

For example, the following set of ED_EXP commands characterises a binary (A-B) three-phase equilibrium (FCC-BCC-LIQ) in a ternary system (A-B-C). It can be used in a POP-file that otherwise only contain experimental information about the ternary system (A-B-C):

```
CREATE_NEW_EQUILIBRIUM 1 0
CHANGE_STATUS COMPONENT A B = ENTERED
CHANGE_STATUS PHASE FCC BCC LIQ=FIX 1
SET_CONDITION P=1E5
EXPERIMENT T=1177:10
COMMENT from A-B
```

Using Stability Conditions

Early in the optimization when parameter values are not so good it is often useful to set the driving force for precipitation of a phase (per mole of components) to make sure that it appears where it should. The DGM condition is very useful for making sure that phases appear where they should. It can be removed when the optimization becomes stable.

The DGM condition is also useful for suppressing phases that appear where they should not appear. Do this by setting the value and the uncertainty to something reasonable. For example, the driving force for precipitation of the BCC phase could be set as follows:

```
DGM(BCC)<-0.1:0.1
```

This produces an error even before BCC becomes stable and the weight of the experiment in question can be adjusted as needed. If you specify that the driving force for the BCC phase should be below 0 (DGM(BCC)<0:1E-4 for example), then the optimization converges

extremely slowly (if at all). With such a sharp error condition, calculating the equilibrium is like finding the minimum point on a lawn that gently slopes towards a rock wall. The optimization keeps bouncing into the wall.

Another useful stability condition is the phase stability function, abbreviated QF. This can be used to specify that a phase is outside the miscibility gap for a solution phase. If $QF(\text{phase})$ is negative, then the phase is inside the miscibility gap; if $QF(\text{phase})$ is positive, then it is outside the miscibility gap.

Grouping Equilibria with Labels

If you have several equilibria describing experiments that you want to be able to treat collectively, you can give all of the equilibria one and the same label.

Use LABEL to give an equilibrium a label. The label must start with the letter A and can only be up to four characters long. For example, you can insert the following command in several equilibria specifications:

```
LABEL ALH
```

During the optimization, you could use this label to, for example, set all the equilibria that have it to the same weight in the ED_EXP module.

Dividing the POP-File into Several Blocks

For two different reasons, you may have to divide your POP-file into different blocks:

- PARROT uses a buffer for storing compiled experimental data. If there is not enough memory in this buffer for storing all the experiments from the POP-file, then the POP-file can be divided into several blocks. When PARROT encounters the end of a POP-file block, it saves the experimental data that has been compiled to PARROT workspace, clears out the memory buffer and then proceeds to read the next block in the POP-file. This goes on until the experimental data from all the blocks have been saved to the PARROT workspace.
- If you want to put equilibria with different sets of components in one and the same POP-file, then you must divide the file up into blocks. Each block should only contain equilibria that all have the same set of components.

To divide the equilibria in the POP-file into different blocks, enter the ["FLUSH BUFFER" on page 298](#) command between two equilibria. This command marks the beginning of new block. When the command is encountered during the compilation of the POP-file, the compilation of the current block is terminated, the equilibria saved to the PARROT workspace file and a new block is initiated. That the buffer is reinitiated means that all functions and constants that were entered in the previous block must be entered again in new block in order to be used.

When editing your experimental data in the ED_EXP module, you can select which block to load and edit using READ_WORKSPACES <block number>. The block before the first instance of FLUSH_BUFFER is block number 1, the block after the first instance and before the second instance is block number 2, and so on.

The Setup File

In this section:

| | |
|---------------------------------------------------|----|
| Creating the Setup File | 29 |
| Defining the System | 29 |
| Entering the Optimizing Variables | 30 |
| Initializing Optimizing Variables in PARROT | 32 |
| Creating the Workspace File | 33 |
| Compiling the POP-file | 33 |
| Returning Control to the Console | 34 |

Creating the Setup File

The second step is to create the setup file. This is an ordinary Thermo-Calc macro file (*.TCM). Typically, your setup file should contain the following:

- A system definition.
- A section where you enter model parameters and optimizing variables.
- A GO PARROT command.
- A section where initial values are assigned to the optimizing variables for the first optimization cycle.
- A `CREATE_NEW_STORE_FILE <filename.par>` which creates the PARROT workspace file onto which the results of your optimization are continuously saved and updated. By default this workspace file has the same filename as the setup file, but with the *.PAR filename extension.
- A `COMPILE_EXPERIMENTS <filename.pop>` command. Since you often encounter syntax errors when you first try to compile a POP-file, it may be useful to execute this command from the console rather than as part of the setup macro file.
- Normally, you also have a ["SET_INTERACTIVE" on page 119](#) at the end of the setup file. This command returns control over Thermo-Calc to the console.

It is possible to interactively execute all these commands one at a time in the console. It may be instructive to enter the commands that would normally go into the setup file interactively while using the on-line help while you are learning to use the PARROT module.

Defining the System

If you have an existing database with information about your system, then you can write the system definition part of your setup file in two different ways.

- If you have an unencrypted user database, then you can define your system by entering DATA module commands directly in the setup file. Use the DATA commands that you normally use to define a system when doing equilibrium calculations in Thermo-Calc Console Mode.
- Define your system by entering DATA module commands directly in the console, then generate a macro file with the GIBBS command `LIST_DATA <name of setup file>.tcm p`. This command saves all the data that has been loaded in the GIBBS workspace as a macro file. This file can then be modified as required into an optimization setup file.

Creating Additional Composition Sets of a Phase

If you need several composition sets of a phase, then these should be created with the GIBBS command `AMEND_PHASE_DESCRIPTION <phase name> composition_sets <composition set number>` in the setup file.



If you add composition sets of a phase after the POP-file has been compiled, the data structure in the workspace is corrupted and you have to recompile the POP-file.

Entering the Optimizing Variables

When you have retrieved the data about your system for the setup file, you must manually enter the model parameters that you want to optimize. This is done using the GIBBS command ["ENTER_PARAMETER" on page 268](#), but when you specify the Gibbs energy expression for the parameter, you enter variables that can be given various values into the expression. It is the values of these variables (and thus, the Gibbs energy of the parameter) that you are optimizing.

How you in detail specify the optimizing variables in your set up file depends on which phase you are trying to optimize and what thermodynamic model that is used in the optimization.

► ["Thermodynamic Models" on page 65](#)

Entering Optimizing Variables in Parameter Specifications

There are ninety-nine predefined variables in the PARROT module which you can use in your optimization. These variables are referred to as `v1`, `v2`, `v3`, ... `v98` and `v 99`. When the GIBBS workspace is initialised, all optimizing variables are set to a fixed numerical value of zero. When you do an optimization, there is always some variable for which you want to evaluate the best value, but you can assign fixed values to optimizing variables too. It is often useful to enter all the variables that you can conceivably want to optimize, and then you can interactively select and change which variable to focus at various stages of the optimization.

The setup file excerpts that follow show how optimizing variables are entered. However, before the optimizing variables are introduced in this example, the following command enters an ionic liquid solution phase (a phase for which you have some experimental information):

```
ENTER_PHASE IONIC_LIQ Y,  
AL+3,ZR+4 ; AL02-1,O-2 ; N N
```

This ["ENTER_PHASE" on page 228](#) command enters a phase called IONIC_LIQ into the GIBBS workspace. This phase is of the type ionic liquid solution, which is specified by type code Y. Such a phase is modelled by the *Ionic Two Sublattice Liquid Model*. The next two arguments specify the two sublattices, in this case the cations AL+3,ZR+4 and the anions ALO2-1,O-2. Components that interact in a sublattice are separated by a comma. The first N at the end means that no additional constituents are added to the phase. The second N means that a list of possible parameters for the phase should not be shown in the console.

There are model parameters that describe the phase which you do not want to optimize, in which case the Gibbs energy expression of the parameter does not contain any optimizing variables.

EXAMPLE 1

For example, the following parameters of the IONIC_LIQ phase do not contain any optimizing variables:

```
ENTER_PARAMETER G(IONIC_LIQ,AL+3:ALO2-1;0) 298.15 +2*GAL2O3_L;  
6000 N  
  
ENTER_PARAMETER G(IONIC_LIQ,AL+3:O-2;0) 298.15 +GAL2O3_L+400000;  
6000 N  
  
ENTER_PARAMETER G(IONIC_LIQ,ZR+4:O-2;0) 298.15 +2*GZRO2L; 6000 N
```

These parameters define the Gibbs energy expressions for three constituents in the constituent array, namely AL+3:ALO2-1, AL+3:O-2 and ZR+4:O-2. The names that occur in these expressions—that is, GAL2O3_L and GZRO2L—are the names of complex functions of temperature that are entered in the GIBBS workspace with the ["ENTER_SYMBOL" on page 231](#) command.

The numbers that frame the Gibbs energy expressions specify the temperature range within which the expression should be applied. In the above, the expressions are applied in a temperature range from 298.15 K to 6000 K.

EXAMPLE 2

In this example, suppose that you want to optimize the model parameter for the ZR+4:ALO2-1 combination, then you could enter the variables V1 and V2 in the Gibbs energy expression for that parameter in the following way:

```
ENTER_PARAMETER G(IONIC_LIQ,ZR+4:ALO2-1;0) 298.15 +GZRO2L  
+2*GAL2O3_L +V1+V2*T; 6000 N
```

You normally have different optimizing variables in different parameters, but in some cases you may want several parameters to vary together, in which case you can use the same variable in the Gibbs energy expressions of several parameters.

Entering Interaction Parameters

For some systems, you have to consider interaction parameters in order to take excess Gibbs energy into account and correctly model the phase. By default, the software uses a Redlich-Kister expression for the excess Gibbs energy. The coefficient is entered after the constituent array when you use the ["ENTER_PARAMETER" on page 268](#) command. In the last section, all the parameters were entered with a coefficient of zero (0).

EXAMPLE

To take account of the excess Gibbs energy, you might enter the following:

```
ENTER_PARAMETER L(IONIC_LIQ,ZR+4:ALO2-1,O-2;0) 298.15 +V11+V12*T;  
6000 N  
  
ENTER_PARAMETER L(IONIC_LIQ,ZR+4:ALO2-1,O-2;1) 298.15 +V13+V14*T;  
6000 N  
  
ENTER_PARAMETER L(IONIC_LIQ,ZR+4:ALO2-1,O-2;2) 298.15 +V15+V16*T;  
6000 N
```

Parameters with interaction coefficients are referred to as *interaction parameters*. The regular parameter has a coefficient of 0. The subregular parameter has a coefficient of 1. It is possible to interaction coefficients up to a value of 9, but you are advised not to use more than three coefficients (that is, with coefficient values of 0, 1 and 2).

Initializing Optimizing Variables in PARROT

Variables that have been entered into Gibbs energy expressions for model parameters in the setup file has to be initialized and given start values before they are optimized.

You have to estimate what start values to give to the optimizing variables based on your knowledge of the system or of relevantly similar systems. There are no general rules for what start values your optimizing variables should have. If you are not able to make any informed estimation about what start values to use, then you may not be able to find a good fit between your experimental data and your calculated results. In this case, it is often best to start the optimization in the so-called alternate mode. In alternate mode, the PARROT module helps you find some reasonable start values for your optimizing variables.

► ["About Alternate Mode" on page 49](#)

Even if you are starting your optimization in alternate mode, you still have to initialize the optimizing variables though (you can all give them a start value of 0).

To initialize an optimizing variable and to give it a start value, use either ["SET_OPTIMIZING_VARIABLE" on page 282](#) or ["SET_SCALED_VARIABLE" on page 283](#). Using SET-OPTIMIZING_VARIABLE results in a scaling factor equal to the current value of the parameter unless the current value is zero, in which case the scaling factor is 1000. This is typically appropriate for enthalpic parameters, but not necessarily for other parameters. The scaling factor is the factor by which the optimizing variable value is varied during the optimization.

EXAMPLE

For example, if you want to optimize the variables V1, V2, V11, V13 and V17, then you could enter the following in the setup file:

```
SET_OPTIMIZING_VARIABLE 1 +43000
SET_OPTIMIZING_VARIABLE 2 -35.2
SET_OPTIMIZING_VARIABLE 11 +72000
SET_OPTIMIZING_VARIABLE 13 +27000
SET_OPTIMIZING_VARIABLE 17 -100000
```

The value given to each optimizing variable (+43000 for variable V1 for example) is also that variable's initial scaling factor. If you want to set the initial scaling factor of a variable to a value that is lower or higher than its start value, then use SET-SCALED_VARIABLE <start value><scaling factor><min value><max value>.

Creating the Workspace File

In the setup file, after the system definition and the entered optimizing variables, use the PARROT command ["CREATE_NEW_STORE_FILE" on page 263](#) to create and save a PARROT workspace file for the system defined in the setup file. For example, the following command saves all current data on system definitions (elements, species, components, phases), symbol definitions (constants, variables, functions, tables) and parameters that are stored in the workspace used by GIBBS, POLY and PARROT into a file called AL2O3-ZRO2.PAR:

```
CREATE_NEW_STORE_FILE AL2O3-ZRO2
```



The experimental information in the POP-file is not saved to this PARROT workspace file.

Compiling the POP-file

At the end of the setup file, use the command ["COMPILE_EXPERIMENTS" on page 261](#) followed by the name of your POP-file to compile the data in that file and save it to the

current PARROT workspace file. Note that you must first have opened or created a new PARROT workspace file before you compile your POP-file. The other argument to the command can typically be given default values with comma signs (,):

```
COMPILE_EXPERIMENTS AL2O3-ZRO2.POP,,,
```

If Thermo-Calc encounters errors in the syntax of the POP-file, then error messages are displayed in the console. Normally, the compilation also stops when syntax errors are encountered. If this happens, then you must correct the errors and recompile the file. It is useful to have two console windows open when you do this. That way, you can use one console for editing the experimental data and another console for compiling and reading any further error messages.

Returning Control to the Console

Put the command ["SET_INTERACTIVE" on page 119](#) at the end of the setup file if you want to return control to the console when the commands in the setup file have all been executed.

Optimizing in PARROT

In this section:

| | |
|-----------------------------------------------------------|----|
| Optimizing the System in PARROT | 36 |
| Changes that Require POP-file Recompilation | 36 |
| Optimization Workflow | 36 |
| Ensuring Computation of all Equilibria | 37 |
| Setting Weights | 38 |
| Optimizing and Evaluating Results | 39 |
| Continuing the Optimization and Resetting Variables | 40 |
| Updating the Set of Optimizing Variables | 42 |
| Reducing the Number of Optimizing Variables | 43 |
| Plotting Intermediate Results | 43 |

Optimizing the System in PARROT

When you have created a POP-file, a setup macro file and (optionally) EXP-files, you should start doing optimization runs interactively in the console. This process can be divided into a number of steps (such as running optimization, evaluating optimization results, modifying weights and models and adding new information), but usually, you have to go through many optimization cycles before achieving a satisfactory fit between calculation results and experimental data.

Typically, it is not obvious when an optimization is finished. You must exercise your judgement about when the fit you have achieved is good enough.



It is possible to interactively change almost everything in the initial setup macro file and in the POP-file. For example, you can add more parameters to be optimized and modify or add more experimental information.

Changes that Require POP-file Recompilation

Some changes that you do interactively in the PARROT module or the ED_EXP sub-module destroys the data structure in the workspace. For example, if you add more composition sets to a phase, then the number of phases actually change and the links break between the experimental data and the thermodynamic models. Note that if the global minimization technique is used in POLY, then new composition sets that corrupts the PARROT workspace may be created automatically. If this happens, then you have to compile the POP-file again.

If you recompile the POP-file, then the experimental equilibria are calculated with the default start values.

Optimization Workflow

Normally, the workflow during an optimization is the following:

1. In the PARROT module, run the setup macro file using ["MACRO_FILE_OPEN" on page 114](#).
2. Go to ED_EXP with ["EDIT_EXPERIMENTS" on page 263](#), use ["READ_WORKSPACES" on page 241](#) to load your experimental data and then execute .
3. If an equilibrium cannot be computed, then this either means that the start values (site fractions, for example) were inappropriate or that the equilibrium cannot be calculated with the current set of parameters. If the latter, then the equilibrium may have to be excluded from the optimization. However, you should make an effort to exclude the possibility that the reason is just that you do not have the appropriate start values for the equilibrium.

-
4. When each equilibrium is either successfully computed or excluded from the calculation, go back to the PARROT module and run the ["OPTIMIZE VARIABLES" on page 277](#) command. Give the number of optimization iterations you want the Thermo-Calc program to carry out as an argument to the command. This number specifies how many different sets of values for the optimizing variables that PARROT tries to fit with the experimental data. It is recommended that you run 0 iterations first to see the discrepancy between the experimental data and the initial calculated results. The current workspace file is automatically updated with the last set of optimized variables and calculated results.
 5. List and evaluate the result of the optimization using ["LIST_RESULT" on page 272](#). Typically, what is of interest in the results are the relative standard deviation of the optimizing variables and the error values in the list of calculated experimental data results. If the relative standard deviation for an optimizing variable is very large, this means that the variable doesn't have any effect on the computed results and that the variable should not be used (you can make PARROT ignore the variable by setting its value to 0 with ["SET_FIX_VARIABLE" on page 280](#)). If the relative standard deviation is close to zero for a variable, then this might indicate that you need to use more variables. When it comes to errors in the calculated equilibrium results, these can be decreased by lowering the weight that PARROT gives the experiment in the calculation (the more weight, the more the experiment affects the calculated results).
 6. Use ["OPTIMIZE VARIABLES" on page 277](#) or ["CONTINUE OPTIMIZATION" on page 262](#) to carry out a new optimization cycle. Go back to step 5 above and continue to do optimization cycles until you judge that there is a good enough fit between your calculated results and your experimental data. It is recommended that you do not only rely on feedback from ["LIST_RESULT" on page 272](#) but also frequently plot various diagrams and compare them visually to some of your experimental data.

Ensuring Computation of all Equilibria

When you have run the setup macro file, you should start by trying to compute all the equilibria that were created when your POP-file was compiled. To do this, you must first go to the ED_EXP submodule, and load the experimental data from the current PARROT workspace file with the `READ_WORKSPACES <block #>` command (normally, the block number is 1).

When you have loaded all equilibria, you should try to compute them all using the ED_EXP command. A list of calculated equilibrium results are shown in the console, but the software is not able to reach an equilibrium for an experiment, then the program cancels the calculations and displays an error message.

The following list shows an example output where the first two experiments in the POP-file have been successfully computed, but an equilibrium is not reached for the third experiment. No other equilibria are computed, since the calculations are aborted when the error occurs.

```
Eq  Lab  Iter Weight Temp  Exp  Fix phases or comments
  1  A1   22   1.   2575.3      IONIC_ FLUORI TETR
  2  A1   18   1.   2156.9      IONIC_ CORUND TETR
*** ERROR 1614 IN QTHISS
*** CONDITIONS CAN NOT BE FULLFILLED
```

When this happens, try to find out why the equilibrium calculation fail. Are the condition start values that you have given the equilibrium inappropriate for example? If you have a similar equilibrium that has already been successfully computed, then you can select the equilibrium that does not work, use the ED_EXP command ["SET_ALL_START_VALUES" on page 178](#) and accept all the suggestions for the site fractions. Alternatively, use TRANSFER_START_VALUE <equilibrium number> to make the currently selected equilibrium inherit the start values of the indicated equilibrium. Run ["COMPUTE EQUILIBRIUM" on page 156](#) again to see if the equilibrium can be computed with the inherited start value.

If you cannot find an explanation of why the equilibrium cannot be computed, then it may be that the experiment is faulty. If so, then this experiment should be excluded from the optimization by being given a weight of 0. You should then run COMPUTE_EQUILIBRIUM again to make sure that all equilibria can be computed. However, experiments that fail to reach equilibria could succeed in doing so if the optimizing variables have other values. It is therefore sometimes worth trying to include experiments later in the optimization process (when the optimizing variables are relatively close to their final values), even if they had to be excluded at its start. In some cases, it might also be appropriate to change the error tolerance for in an experiment (using the ED_EXP command ["EXPERIMENT" on page 296](#)).



You must save the PARROT workspace with ["SAVE_WORKSPACES" on page 305](#) before you exit the ED_EXP module.

Setting Weights

To change the weight of an experiment, first enter the ED_EXP module from PARROT using ["EDIT_EXPERIMENTS" on page 263](#). Then use the ["SET_WEIGHT" on page 316](#) command to set the weight for a specific equilibrium (equilibrium number 3 for example), for a range of equilibria (the equilibria 10–19) or all the equilibria that have a certain label (such as all the equilibria with the label A1). To save the new weight(s), use ["SAVE_WORKSPACES" on page 305](#).

By default, all the experimental information in your POP-file is treated equally: each experiment has a weight of 1. However, experiments that you excluded because they did not reach equilibrium now have a weight of 0. The higher the weight of an experiment is, the more Thermo-Calc tries to ensure that the computed result fits the condition measured in that experiment.

The contribution of an experiment's error to the sum of errors is multiplied by the square of the weight set for that experiment. In other words, if you want to cut the error of an experiment with weight 1.0 by half, then you should use a weight of 0.7. This makes the experiment's error 0.49. Setting the weight to 1.4 instead makes the error twice as large (1.96).

Note that if you use ["READ WORKSPACES" on page 241](#) after you have changed weights on the experiments, your changes are lost unless you have saved those changes. In the ED_EXP module, you can get a list of all the experiments in the console if you first read the experimental data from the workspace file (with READ_WORKSPACES) and then use ["LIST ALL EQUILIBRIA" on page 300](#).

Optimizing and Evaluating Results

When you have ensured that all the experimental data points can reach equilibrium, go back to the PARROT module and use ["OPTIMIZE VARIABLES" on page 277](#) <number of iterations> with 0 iterations. Present the result of this initial optimization by using ["LIST RESULT" on page 272](#).

When evaluating the optimization results, the most important information is found in the list of experiments at the end of the listed results. The rightmost column shows the difference between the value of the experimental data and the value computed by Thermo-Calc in the last optimization cycle.

The following shows part of list of experiments in the output of a LIST_RESULT command:

| | | | | |
|-----------------------|-------------|----------|-------------|---------|
| 106 ACR(B)=0.34 | 0.3127 | 2.89E-02 | -2.7282E-02 | -0.9444 |
| 107 ACR(B)=0.23 | 0.2085 | 2.89E-02 | -2.1522E-02 | -0.7450 |
| 108 ACR(B)=0.12 | 0.1042 | 2.89E-02 | -1.5761E-02 | -0.5455 |
| 110 HMR(LIQUID)=-1964 | 3.6380E-12 | 5.00E+02 | 1964. | 3.928 |
| 111 HMR(LIQUID)=-3500 | 0.000 | 5.00E+02 | 3500. | 7.000 * |
| 112 HMR(LIQUID)=-4588 | 0.000 | 5.00E+02 | 4588. | 9.176 * |
| 113 HMR(LIQUID)=-5239 | 7.2760E-12 | 5.00E+02 | 5239. | 10.48 * |
| 114 HMR(LIQUID)=-5454 | -3.6380E-12 | 5.00E+02 | 5454. | 10.91 * |
| 115 HMR(LIQUID)=-5233 | 1.8190E-12 | 5.00E+02 | 5233. | 10.47 * |
| 116 HMR(LIQUID)=-4575 | -1.8190E-12 | 5.00E+02 | 4575. | 9.150 * |
| 117 HMR(LIQUID)=-3481 | -1.8190E-12 | 5.00E+02 | 3481. | 6.962 * |
| 118 HMR(LIQUID)=-1950 | 0.000 | 5.00E+02 | 1950. | 3.900 |

PARROT:

The experiments for which the optimization has not found a good fit are marked with an asterisk (*) or a hash sign (#) in the rightmost column. An asterisk in this column indicates that the experiment has an error that is larger than the error tolerance and a hash sign indicates that the error is much larger. The error tolerance depends on the degree of accuracy set for that particular piece of experimental information. The error values are presented in the next to rightmost column.

Note that if you are optimizing in *alternate mode*, then you usually do not need to change the weights for the experiments. Instead, you can simply run OPTIMIZE_VARIABLES again, specifying, say, thirty iterations, evaluate the results again, and continue in that way until you are satisfied with the results.

► ["About Alternate Mode" on page 49](#)

The Critical Set of Experiments

The set of weighted experiments that you end up with as a result of your optimization is referred to as the *critical set* of experiments. When you work to determine this set and the weights of the experiments, the following factors should be reflected in both the selection of experiments and the weights of those experiments:

- The reliability of the experimental technique.
- The extent of agreement/disagreement between independent measurements of the same quantity.
- The extent of agreement/disagreement between data obtained with different experimental methods.

Continuing the Optimization and Resetting Variables

To continue the optimization after you have used ["OPTIMIZE_VARIABLES" on page 277](#), you can either use this command and enter `<Number of iterations>` again or ["CONTINUE OPTIMIZATION" on page 262](#) `<Number of iterations>`.

If you use CONTINUE_OPTIMIZATION, then PARROT continues the optimization using the same Hessian matrix. If the optimization is going well but you run out of iterations, then continuing with the same Hessian matrix may be useful.

As before, use ["LIST_RESULT" on page 272](#) to inspect the fit between the calculated and the experimental values for your experiments. If necessary, adjust the weights of the experiments again in the ED_EXP module. You may even discover that you have to exclude additional experiments from the optimization.

Besides looking at the rightmost column in the list of experiments (that is produced when you use LIST_RESULT), it is also useful to look at the *sum of squares* of the errors of all the variables. This is shown in the output of OPTIMIZE_VARIABLES and CONTINUE_OPTIMIZATION. This sum should be as low as possible.

The following shows part of the output that you get when using LIST_RESULT:

```
== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.   VALUE           START VALUE      SCALING FACTOR    REL.STAND.DEV
V1      6.94641846E+05    4.30000000E+04    4.30000000E+04    1.42299558E+00
V2     -3.32619842E+02   -3.52000000E+01   -3.52000000E+01   7.91369573E-01
V11     8.37422071E+04    7.20000000E+04    7.20000000E+04    2.02212692E-01
V13     2.65253341E+04    2.70000000E+04    2.70000000E+04    1.45201828E-01
V17    -3.66637428E+05   -1.00000000E+05   -1.00000000E+05    8.04279315E-01

NUMBER OF OPTIMIZING VARIABLES :    5
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM  3.50196879E+05 TO  3.49096720E+05
DEGREES OF FREEDOM   14.  REDUCED SUM OF SQUARES  2.49354800E+04
```

In the example you can see that the sum of squares have decreased slightly. (The final sum of squares that you get after an optimization run is also presented directly in the output from OPTIMIZE_VARIABLES and CONTINUE_OPTIMIZATION.) As long as the sum of squares figure is decreasing, the optimization is working as it should.

When your calculated results have been improving for a while, that is, when the sum of squares has been decreasing, and you are confident that you are making definitive progress, then you should use the PARROT command ["RESCALE VARIABLES" on page 278](#) to reset the starting values of the optimizing variables to their current values. When you do this, the start values and scaling factors of the optimizing variables (shown in the table's third column in the preceding screen shot), are all set to the current values (shown in the table's second column).

If your optimization is not going well, then you may want to reset the values of your optimization variables to their current start values. To do this, use ["RECOVER VARIABLES" on page 278](#).

After rescaling the variables, continue the optimization using OPTIMIZE_VARIABLES again. Cycle through calls of the commands OPTIMIZE_VARIABLES/CONTINUE_OPTIMIZATION, CONTINUE_OPTIMIZATION, RESCALE_VARIABLES and OPTIMIZE_VARIABLES again until your set of optimizing variables does not seem to improve anymore. Even when it seems to you that you have reached this point, it is recommended that you use OPTIMIZE_VARIABLES/CONTINUE_OPTIMIZATION a few extra times to make sure that the variable values cannot be further improved, that is, that the sum of squares of the errors of all the

variables cannot be reduced further. If the final solution is repeatedly calculated after the same number of iterations and reaching the same result, then it is generally reasonable to accept the current variable values.

Updating the Set of Optimizing Variables

Besides evaluating the fit between the calculated results and the experimental data, you should also ensure that you have the right number of optimizing variables. If you have too many or too few optimizing variables, then you may not be able to use your model to accurately extrapolate thermodynamic properties in a wide range of temperature, pressure and composition conditions.

With more optimization parameters, the sum of errors usually decrease, but the parameters also tend to become less precisely determined. A measure of this precision is the Relative Standard Deviation (RSD) of each optimizing variable. However, the RSD is only significant if you have used ["RESCALE VARIABLES" on page 278](#) followed by an optimization which converges and the values of the variables do not change much. The RSD tells you how much the parameter can be changed in either a positive or in a negative direction without changing the reduced sum of errors with more than one unit.

A large RSD value thus means that the parameter has not been determined well.

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

| VAR. | VALUE | START VALUE | SCALING FACTOR | REL.STAND.DEV |
|------|-----------------|-----------------|-----------------|----------------|
| V1 | 2.01820948E+04 | 2.01874462E+04 | 2.01874462E+04 | 2.60519742E-02 |
| V2 | -2.90936164E+01 | -2.90969472E+01 | -2.90969472E+01 | 1.41576516E-02 |
| V11 | -2.18127453E+04 | | | |
| V12 | 1.55559524E+01 | | | |
| V15 | 2.36701148E+04 | 2.37258719E+04 | 2.37258719E+04 | 1.00528931E-01 |
| V16 | -7.56541897E+00 | -7.64417807E+00 | -7.64417807E+00 | 3.17218507E-01 |
| V17 | 3.00342429E+03 | 3.02274918E+03 | 3.02274918E+03 | 2.60675550E-01 |
| V19 | 2.20133190E+04 | 2.14534347E+04 | 2.14534347E+04 | 6.92923849E-01 |
| V20 | -6.72498276E+00 | -6.31334932E+00 | -6.31334932E+00 | 1.79242248E+00 |

NUMBER OF OPTIMIZING VARIABLES : 7

ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO

THE SUM OF SQUARES HAS CHANGED FROM 1.51360340E-01 TO 1.44420287E-01

DEGREES OF FREEDOM 18. REDUCED SUM OF SQUARES 8.02334928E-03

If such a significant RSD has a value larger than 1, then this typically means that you are using too many optimizing variables. However, the RSD values also depend on the weighting of the experiments, so it is sometimes possible to reduce the RSD by changing weights.

The RSD should not be too low either. If one or more of them is very close to 0, then this suggests that you are trying to optimize the system with too few optimizing variables. You can add optimizing variables interactively using ["ENTER_PARAMETER" on page 268](#) in GIBBS. However, it is recommended that you add a sufficient number of variables in the setup file from the start so that do not need to do this. You can fix variables to a value of 0 until you discover that they are needed.

Besides the RSD, you should also keep an eye on the variable values themselves (shown in the VALUE column, next to the leftmost column in the table shown in the preceding screenshot). If the value of a variable is in the order of $1E5$ or higher and this variable has been put in the temperature-independent part of an interaction parameter's Gibbs energy expression, then you may not have the right weights on your experiments or you are using too many optimizing variables. This is also typically the case if a variable with a value in the order of 10 or more (per mole atoms) is in the temperature-dependent part of the Gibbs energy expression of an interaction parameter. Such a high parameter value may lead to inverted miscibility gaps or re-stabilisation of a phase at high temperature. It is important to keep an eye on this since the temperature-independent and the temperature-dependent interaction parameter often varies together. If the temperature-dependent interaction parameter cannot be reliably determined, you may have to fix its value.

Note that even if you have found a good enough fit between calculated and experimental values after an optimization run, a parameter value may suddenly start to change by several orders of magnitude when you use ["OPTIMIZE_VARIABLES" on page 277](#) is used again. If this happens, then careful reconsideration of the weighting of the experiments of the set of optimizing variables is required. However, when the optimization has converged and the parameter values remain stable after repeated use of OPTIMIZE_VARIABLES, this should usually not happen.

Reducing the Number of Optimizing Variables

If you have one or more optimizing variables with RSD larger than 1, then you should remove one or more of the variables by setting them to a value of 0, or alternately, set them to a reliably estimated value (estimated based on, for example, semi-empirical methods).

To fix an optimizing variable to certain value, use the PARROT command SET_FIX_VARIABLE <variable number> <value>.

Plotting Intermediate Results

It is typically not sufficient to look at the plain text output of ["LIST_RESULT" on page 272](#) to reliably judge how the optimization is progressing. Plotting a phase or property diagram of the system you are optimizing using the POLY and POST modules is often very useful.

It is recommended that you create a macro file for plotting the diagram since you probably want to repeatedly plot the diagram as you progress with the optimization. This macro file can then be called directly from the PARROT module with the ["MACRO_FILE_OPEN" on page 114](#) command.

Superimposing Experimental Data from EXP-files

If you create one or several EXP-files based on the experiments in your POP-file, you can visually compare the fit your plot and the experimental data you are optimizing the system against. An EXP-file contains data points specified in the DATAPLOT format. You could make an EXP-file for each type of data that you are using in the optimization.

Use the POST command ["APPEND_EXPERIMENTAL_DATA" on page 353](#) to superimpose the data points in an EXP-file on a phase or property diagram that you have plotted. For example, to put the experimental data points from a file entitled DP.EXP onto a plotted diagram, you could enter the following:

```
APPEND_EXPERIMENTAL_DATA Y DP.EXP 0 1
```

Such a command call tells Thermo-Calc to superimpose the data points in dataset 1 of DP.EXP onto the plot in the Console Results window, but not to impose any information about axis scaling, labels and other information which is normally found in the prologue of the DP.EXP file.

The POST command ["QUICK_EXPERIMENTAL_PLOT" on page 362](#) can also be used to superimpose data points on a plotted phase or property diagram.

► *DATPLOT User Guide* included with this documentation set.

Finalizing the Optimization

In this section:

| | |
|------------------------------------------------|----|
| Finishing the Optimization | 46 |
| Rounding off Optimizing Variable Values | 46 |
| Updating the Database File | 46 |
| Creating a Database File | 47 |
| Updating the Setup File and the POP-file | 47 |

Finishing the Optimization

When to stop optimizing is a matter of judgement. It is rarely the case that you finish optimizing a system with the feeling that it cannot be improved.

The final step is to update your files with the final results. Besides updating your database file (or alternatively, creating a new database file), it is advised that you also update your setup and POP-files with the final weights and optimizing variable values.

Rounding off Optimizing Variable Values

When you save the optimizing variable values, it is important that you round off the values correctly. When you have a metallic system, it is usually best to keep whatever number of decimal digits that you need to make less than one J/mol difference at 1000 K. When you have an aqueous system or a system that you are optimizing based on data from very different temperature ranges, then this is not always the only appropriate guideline. However, rounding off the values in such a way that it gives a difference that is larger than one J/mol may lead to differences in the phase diagram.

Another approach you can take when rounding off variable values is by progressively fixing the value of more and more of the variables. This allows you to round-off all but one of the variables values so that each only has a few significant digits. Variables whose values have been rounded off in this way are easier to handle compared with those that are rounded off so that they continue to have many significant (non-zero) digits.

To round off the variable values according to this second approach, first use ["SET_FIX VARIABLE" on page 280](#) to set the variable(s) with the highest RSD to a rounded off value (such as, say, 0.4). When you then re-optimize using ["OPTIMIZE VARIABLES" on page 277](#), the sum of errors changes. However, you should get almost exactly the same sum of errors as before after you rescale the variable values using ["RESCALE VARIABLES" on page 278](#). (If the sum of errors is different, then this means that the variable with the highest RSD was not rounded off in a good way.) If you successfully round off the first variable value, then continue to round off the optimizing variable which now has the highest RSD. Continue doing this until you have fixed all but one of the optimizing variables to their rounded-off values. The final sum of errors that you get after having fixed the variable values should not deviate significantly from the initial sum of errors you had before starting to round-off the variable values.

Updating the Database File

To update the database file (with filename extension TDB) open it in a text editor and enter or update each of the parameters that you have optimized.

For example, suppose you have the following command in your setup file:

```
ENTER_PARAMETER L(IONIC_LIQ,AL+3,ZR+4:O-2;0) 298.15 +V17; 6000 N
```

If you then end up with a value for optimizing variable V17 of -100000, then you should enter the following under the IONIC_LIQ phase in the database file:

```
PARAM L(IONIC_LIQ,AL+3,ZR+4:O-2;0) 298.15 -100000; 6000 N REF !
```



If you often need to round-off the optimizing variable value in some way, see ["Rounding off Optimizing Variable Values" on the previous page](#).

When you have updated or entered the parameters that you optimized, save the database file.

Creating a Database File

In some circumstances you may want to save all the information about your system into a new database file. To do this, go to the GIBBS module and use LIST_DATA <Filename> N. This creates a new user database file that contains all the information about the system that is in the workspace.

The N-argument tells the ["LIST_DATA" on page 235](#) command to save the output into database file rather than some other type of file, such as a macro file for example. Note that the output database file that you get from LIST_DATA have to undergo some manual editing before it can be used as proper database file.

Updating the Setup File and the POP-file

It may be useful for you to be able to recreate your optimization from scratch. It is therefore recommended that you do the following when you are done with the optimization:

- Update your POP-file so that it contains the weights of your critical set of experiments. Use ["SET_WEIGHT" on page 316](#) to set the weights directly in the POP-file. You may also have to use ["SET_START_VALUE" on page 187](#) for some conditions in the POP-file. Otherwise, you may not be able to compute the equilibria with .
- Copy the final values of your optimizing variables and set them as start values of the variables in the setup macro file (with ["SET_FIX_VARIABLE" on page 280](#)).



It is important that you round off the values of the optimizing variables correctly. See ["Rounding off Optimizing Variable Values" on the previous page](#). When you have done this, you can run the setup macro file to recreate the final result of the optimization.

Alternate Mode

In this section:

| | |
|-------------------------------------------------|----|
| About Alternate Mode | 49 |
| Optimizing in Alternate Mode | 50 |
| Preparing the POP-file for Alternate Mode | 50 |
| Examples of SET_ALTERNATE_CONDITION | 50 |

About Alternate Mode

To turn Alternate Mode ON or OFF, use the PARROT command ["SET_ALTERNATE_MODE" on page 279](#).

When you have one or more multi-phase equilibria (that is, with the fixed phase-status) in your POP-file and the optimizing values lack appropriate starting values (such as the default value of 0 for example), then Thermo-Calc may not be able to compute the equilibria for the experiments. In these cases, a common tangent cannot be found, that is, a state where the chemical potentials for all components are the same in all phases cannot be found. A common tangent may not exist or it be found at the wrong composition or temperature given the initial set of model parameters.

If you are not able to estimate reasonable starting values for the optimizing variables, then this problem can be overcome by initially running your optimization in alternate mode. The alternate mode in PARROT module should help you find reasonable starting values for the optimizing variables. Note that you are only supposed to use alternate mode in the beginning of the optimization. Once you have achieved a reasonable fit between calculated results and experimental data, turn off alternate mode and calculate all equilibria again in the normal mode.

In alternate mode, PARROT modifies multi-phase equilibria so that the chemical potentials for each stable phases is calculated separately. For example, consider the following experimental equilibrium:

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE LIQ FCC=FIX 1
SET_CONDITION T=1000 P=1E5
EXPERIMENT X(LIQ,B)=.2:.01 X(FCC,B)=.1
```

When PARROT optimizes in alternate mode, the computation of this equilibrium is done by way of the following two calculations:

```
CHANGE_STATUS PHASE LIQ=FIX 1
SET_CONDITION T=1000 P=1E5 X(LIQ,B)=.2
CHANGE_STATUS PHASE FCC=FIX 1
SET_CONDITION T=1000 P=1E5 X(FCC,B)=.1
```

The difference between the chemical potentials in every pair of phases is calculated and PARROT tries to adjust the parameters of the phases so that these differences are minimized. In other words, PARROT tries to make the chemical potentials equal in all phases. For PARROT to be able to do this, some additional information about the experimental multi-phase equilibria is required, at least for all invariant equilibria.

Optimizing in Alternate Mode

When you are optimizing in the alternate mode, you usually do not need to enter the ED_EXP module and manually change the weights of experiments that the computed results have not been fitted well with. Instead, after using ["OPTIMIZE VARIABLES" on page 277](#) initially with no iterations, and listing the result with ["LIST_RESULT" on page 272](#), simply run OPTIMIZE_VARIABLES again specifying, say, thirty iterations. Continue to optimize until your optimization seems to be going in the right direction, then set the optimizing variables' starting values to their current values use ["RESCALE VARIABLES" on page 278](#) before you turn alternate mode off by answering N at the ["SET_ALTERNATE_MODE" on page 279](#) prompt.

Preparing the POP-file for Alternate Mode

Information in your POP-file that concerns equilibria with ENTERED or DORMANT phases is ignored when you optimize in alternate mode.

To use the alternate mode, ensure that there is enough information about each phase in a given equilibrium. In addition to the temperature and pressure of the system, you should specify the composition of all phases in a given equilibrium. This is done with, ["SET_CONDITION" on page 181](#), ["EXPERIMENT" on page 296](#) or ["SET_ALTERNATE_CONDITION" on page 307](#).

If both compositions of a binary tie-line have been measured, then you could specify this in the POP-file in the following way:

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE FCC BCC=FIX 1
SET_CONDITION P=1E5 T=1000
EXPERIMENT X(BCC,B)=.2:.01 X(FCC,B)=.3:.01
```

This equilibrium could be calculated with alternate mode without any modification. The compositions specified with the experiment command is used as condition when the thermodynamic properties of each phase are calculated.

Examples of SET_ALTERNATE_CONDITION

The following topics demonstrate how ["SET_ALTERNATE_CONDITION" on page 307](#) is used to prepare different kinds of equilibria for optimization in alternate mode.

SPECIFYING THE COMPOSITION OF ONE SIDE OF A BINARY TIE-LINE

If only one side of the tie-line has been measured, then you must provide an estimate of the

composition of the other phase. You can make such an estimate with SET_ALTERNATE_CONDITION. This command has no effect unless alternate mode is turned on. The equilibrium described could thus be specified in the following way:

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE FCC BCC=FIX 1
SET_CONDITION P=1E5 T=1000
EXPERIMENT X(BCC,B)=.2:.01
SET_ALTERNATE_CONDITION X(FCC,B)=.3
```

When the alternate mode is turned on, the composition given by the SET_ALTERNATE_CONDITION command is used for the FCC phase. The properties of the BCC phase is calculated using the composition specified by experiment as a condition.

SPECIFYING THE COMPOSITIONS OF A THREE-PHASE EQUILIBRIUM

If you have a three-phase equilibrium in your POP-file, then one of its compositions can be specified as experimentally determined, while two can be provided as alternate conditions:

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE FCC BCC LIQ=FIX 1
SET_CONDITION P=1E5
EXPERIMENT T=912:5 X(LIQ,B)=0.2:.02
SET_ALTERNATE_CONDITION X(FCC,B)=0.1 X(BCC,B)=.4
```

SPECIFYING THE COMPOSITION OF A STOICHIOMETRIC PHASE

When you specify the composition of stoichiometric phase with SET_ALTERNATE_CONDITION, the value must be given with at least seven decimal digits, as in the following example:

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE LIQ A2B=FIX 1
SET_CONDITION P=1E5 X(LIQ,B)=0.2
EXPERIMENT T=992:5
SET_ALTERNATE_CONDITION X(A2B,B)=.6666667
```

Entering Other Experiments in the POP with Alternate Mode

The following table shows some additional examples of how to enter different kinds of experiments in the POP-file when you are using the alternate mode.

| Example | ED_EXP commands |
|--------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Two-phase equilibrium: The melting temperature of an Au-Cu alloy | CHANGE_STATUS PHASE LIQUID FCC=FIX 1 SET_CONDITION X(FCC,CU)=0.14 P=1E5 EXPERIMENT T=970:2 SET_ALTERNATE_CONDITION X (LIQUID,CU)=0.16 |
| Invariant equilibrium experiment: A three-phase equilibrium in a binary system | CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC BCC LIQUID=FIX 1 SET_CONDITION P=1E5 EXPERIMENT T=912:5 SET_ALTERNATE_CONDITION X(FCC,B)=0.1SET_ ALTERNATE_CONDITION X(BCC,B)=0.4SET_ALTERNATE_CONDITION X (LIQ,B)=0.2 |
| Ternary system, with two compositions measured (both with uncertainty 0.02) | CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC BCC=FIX 1 SET_ CONDITION T=1273 P=1E5 SET_CONDITION X(FCC,B)=0.1:0.02 EXPERIMENT X (FCC,C)=0.12:.02 SET_ALTERNATE_CONDITION X(BCC,B)=0.17 SET_ ALTERNATE_CONDITION X(BCC,C)=0.07 |

Troubleshooting

During an optimization, you are likely to run into many different problems and challenges. This topic gives some general guidelines that can help avoid common mistakes and problems.

In this section:

| | |
|------------------------------------------------------|----|
| Useful Guidelines | 54 |
| Excluding and Including the Correct Equilibria | 55 |
| Conflicting Data | 56 |

Useful Guidelines

The following rules of thumb are generally good to adhere to when you are planning and executing an optimization:

- Do not use data from thermochemical tables of unknown origin.
- Use experimentally determined properties; avoid converted quantities.
- Carefully estimate the accuracy of the experiments.
- Correct systematic errors (by adjusting a temperature scale for example).
- Use negative information such as, for example, the information that a phase should not be stable in a composition or temperature region.
- With a hundred activity measurements in a system but only ten composition points from the phase diagram, it is often appropriate to decrease the weights on the activity experiments.
- If you initially exclude any intermediate phases to only optimize the liquid and the terminal or end-member phases for the pure components, then it is often useful to compute a metastable phase diagram with just these phases. In the metastable phase diagram, the metastable solubility lines should not have any strange kinks or turns. Such a diagram is often also useful to compute at later stages in the optimization.
- When you have fitted the liquid phase and some solution phases reasonably well, then you can fix the optimizing variables that characterise these phases. You can then go on and optimize the variables for the intermediate phases.
- Phases with miscibility gaps are always difficult to optimize. Try to keep control of the miscibility gaps by using real or estimated experimental information. (Note that it is not possible to calculate the top of a miscibility gap as a single equilibrium.)
- Phases with order/disorder transformation are often difficult to optimize. It may be difficult to find the right start values on the optimizing variables. The TABULATION module can be useful sometimes. Properties for specified site fractions can be calculated in the TABULATION module. This is not possible in the POLY module since this module only calculates for equilibrium site fractions. The ordered state may also disappear during the optimization of these phases. If this happens, you may be able to add an experiment that controls the state of order.
- Only use the alternate mode to find an initial set of model parameters that can then be make it possible to calculate the experimental equilibria in the normal mode.
- When you have achieved a satisfactory fit between calculated results and experimental data with an appropriate number of optimization variables, perform a couple of final optimization runs to make sure that your results are stable.

- Make sure that the values of the optimizing variables keep within a reasonable range. If a variable starts to change several orders of magnitudes, then you must consider whether you have the right weights on the experiments and whether you are using too many optimizing variables.

GES5 and GES6 Calculation Engine Version

As of Thermo-Calc version 2019b, the default calculation engine is set to GES6. For PARROT optimization and POURBAIX module users, you need to use GES5. When you try to enter these modules, you are instructed to switch to GES5 using the SET_GES_VERSION command.

▶ ["About the Gibbs Energy System \(GES\) Module" on page 36](#)



To globally set the default from GES6 back to GES5, go to the **Tools → Options** → ["General" on page 37](#) tab and click **Version 5** for the *Preferred Gibbs Energy System* setting. The ["SET_GES_VERSION" on page 118](#) Console Mode command is used to change GES versions for a single Thermo-Calc session.



Contact Thermo-Calc Software AB at info@thermocalc.com for more information about the changes or if you encounter any issues you think are related to the new version of the calculation engine.

Excluding and Including the Correct Equilibria

Use as few experiments as possible initially to get a reasonable overall fit. It is generally best to first focus on the invariant equilibria, as well as metastable states that can be estimated by excluding some phases. Crucially, any experiments for which the computed results are clearly faulty should be excluded from the final critical set, while all important invariant equilibria are calculated and included in this critical set.

If you cannot compute some invariant equilibria with intermediate phases, then it may be best to first exclude those phases from the optimization and only optimize the liquid and the most important solution phases. After you have obtained reasonable results for these phases, you can enter the intermediate phases back in again. With the variables for the optimized liquid and solid phases set fixed, you can finally optimize the intermediate phases.

Conflicting Data

It is important that you do not include conflicting sets of data at the same time during an optimization. After all, if they are genuinely conflicting, then at least one of the sets must be incorrect. If you have conflicting sets of data, then only use one of these sets at a time together with the rest of the data. Often, the optimization makes it clear which dataset coheres best with the other information that is available about the system.

Sometimes, conflicting data cannot be detected directly. For example, you may have activity data which is inconsistent with solubility data from the phase diagram. This would be indicated by large errors in the fit when both the activity data and the solubility data are included. To find these inconsistencies, let alone correct the errors, you may thus have to optimize with some datasets excluded.

Experiments and Experimental Data

These topics contain examples of different kinds of equilibria in different kinds of systems. They are intended to help you figure out how to use various kinds of experimental data when creating POP-files. The topics that follow contain examples how to enter various kinds of experimental data into a POP-file.

In this section:

| | |
|----------------------------------------------------------------|----|
| Phase Diagram Data | 58 |
| Data for Individual Compounds | 59 |
| Single Phase Mixing Enthalpies or Partial Enthalpies | 60 |
| Enthalpies of Formation and Enthalpies of Reactions | 61 |
| Chemical Potentials via EMF Measurements | 61 |
| Driving Force for Metastable Phases | 62 |
| Pressure-Temperature-Volume EOS Data | 62 |
| Crystal Structure, Lattice Parameters and Site-Occupancy | 63 |
| Magnetism and Other Atomistic Properties | 63 |
| Data About Systems of Different Orders | 64 |

Phase Diagram Data

P-T-X phase diagram data for binary and ternary systems, or systems of even higher order can be used in the POP-file. This includes data of the following types:

- Data about the temperature- and composition-dependence of various properties (obtained from differential thermal analysis (DTA) measurements for example), including enthalpy, lattice parameter, dilatometric length, electronic conductivity and magnetic susceptibility;
- Data about reaction types (invariant/monovariant) and phase relations obtained from qualitative or quantitative metallographic studies;
- Data about phase amounts or compositions obtained from microprobe measurements (using X-ray spectroscopy or transmission electron microscopy (TEM));
- Data about the positions or directions of two-phase tie-lines and three-phase equilibria for ternary systems.

EXAMPLE

The following table shows a POP-file excerpt that demonstrates how some kinds of phase diagram data can be entered:

| Example | ED_EXP commands |
|-------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| Solidus (melting temperature) of an Au-Cu alloy | <pre>CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE LIQUID FCC=FIX 1 SET_CONDITION X(FCC,CU)=0.14 P=1E5 EXPERIMENT T=970:2</pre> |
| Three-phase equilibrium in a binary A-B system | <pre>CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC BCC LIQUID=FIX 1 SET_CONDITION P=1E5 EXPERIMENT T=912:5</pre> |
| Congruent transformation in a binary A-B system | <pre>CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE BCC LIQUID=FIX 1 SET_CONDITION P=1E5 X(BCC,B)-X(LIQ,B)=0 EXPERIMENT T=1213:10</pre> |
| Tie-line in a ternary A-B-C system | An uncertainty factor is set not only for the experimental measurement, but also for the X(FCC,B) condition. The factor is 0.02. |

| Example | ED_EXP commands |
|---------|-----------------------------------------------------------------------------------------------------------------------------------------------------|
| | <pre> CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC BCC=FIX 1 SET_CONDITION T=1273 P=1E5 X(FCC,B)=0.1:0.02 EXPERIMENT X(FCC,C)=0.12:.02 </pre> |

Data for Individual Compounds

You can use data about individual components in the POP-file. Such data includes activity, heat capacity, heat content, entropy, Gibbs energy of phase transformations, heat of transition and heat of melting.

EXAMPLES

| Example | ED_EXP commands |
|---------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Carbon activity data in the fcc phase | <pre> CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC_A1=FIX 1 CHANGE_STATUS PHASE GRAPHITE=D SET_REFERENCE_STATE C GRAPHITE,,,, SET_CONDITION P=101325 T=1273 X(MN)=0.03 SET_CONDITION X(C)=0.03 EXPERIMENT ACR(C)=0.29:5% </pre> |
| Ln(activity coefficient for O) | <pre> CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE IONIC_LIQ=FIX 1 CHANGE_STATUS PHASE GAS=D SET_CONDITION X(O)=0.02 T=1523 P=101325 SET_REFERENCE_STATE O GAS,,,, ENTER_SYMBOL FUNCTION LNFO=LOG (ACR (O) /X (O)); EXPERIMENT LNFO=-1.5:0.01 </pre> |
| Entropy at 298.15 K of Cu2O | <pre> CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE CU2O=FIX 1 CHANGE_STATUS PHASE CUO=FIX 0 SET_CONDITION P=101325 T=298.15 EXPERIMENT S=92.36:1 </pre> |
| Gibbs energy of formation of NiAl2O4 | <pre> CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE SPINEL=ENT 1 </pre> |

| Example | ED_EXP commands |
|-----------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | CHANGE_STATUS PHASE FCC O2GAS=DORM SET_REFERENCE_STATE NI FCC,,,, SET_REFERENCE_STATE AL FCC,,,, SET_REFERENCE_STATE O O2GAS,,,, SET_CONDITION P=101325 T=1000 N(NI)=1 N(AL)=2 SET_CONDITION N(O)=4 EXPERIMENT GM=-298911:5% |
| Heat capacity of MgFe2O4 | CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE SPINEL=ENT 1 SET_CONDITION P=101325 N(Fe)=2 N(Mg)=1 N(O)=4 SET_CONDITION T=800 ENTER_SYMBOL FUNCTION CP=H.T; EXPERIMENT CP=207:5% |
| Heat content (H-H298) for MnFe2O4 | CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE SPINEL=ENT 1 SET_CONDITION P=101325 T=298.15 N(Mn)=1 N(Fe)=2 SET_CONDITION N(O)=4 ENTER_SYMBOL VAR H298=H; ENTER_SYMBOL FUN HMNFE2O4=H-H298; CREATE_NEW_EQUILIBRIUM 2 1 CHANGE_STATUS PHASE SPINEL=ENT 1 SET_CONDITION P=101325 N(Mn)=1 N(Fe)=2 N(O)=4 SET_CONDITION T=400 EXPERIMENT HMNFE2O4=16610:5% |

Single Phase Mixing Enthalpies or Partial Enthalpies

You can use calorimetric data for mixing in the POP-file. This data could be the result of, for example, drop calorimetry or scanning calorimetry. This includes data about, for example, enthalpy of mixing of liquids, series of mixing-enthalpy and about partial enthalpy. Information about enthalpies of mixing can also be derived from theoretical principles using special quasi-random structures (SQSs).

| Example | ED_EXP commands |
|----------------------------------------------------------|----------------------------------------------------------------------------------------------|
| Enthalpy of mixing in the liquid state of an Au-Cu alloy | CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE LIQUID=FIX 1 SET_CONDITION T=1379 P=1E5 |

| Example | ED_EXP commands |
|---------|--------------------------------------------------------------------------------------------------------------------------------------------|
| | <pre> SET_CONDITION X (LIQUID,AU)=0.0563 SET_REFERENCE_STATE AU LIQ * 1E5 SET_REFERENCE_STATE CU LIQ * 1E5 EXPERIMENT HMR=-1520:200 </pre> |

Enthalpies of Formation and Enthalpies of Reactions

You can use calorimetric data for phase transformations in the POP-file. This data could be the result of, for example, direct-reaction calorimetry, solution calorimetry or combustion calorimetry. Information about enthalpies of formation can also be derived from theoretical principles.

EXAMPLES

| Example | ED_EXP commands |
|----------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Enthalpy of melting of the eutectic in the Al ₂ O ₃ -ZrO ₂ binary (J/g) | <pre> CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE CORUNDUM ZRO2_TETR=FIX 0 CHANGE_STATUS PHASE IONIC_LIQ=ENT 1 SET_CONDITION P=101325 N=1 LNAC(O)=-80 SET_REFERENCE_STATE ZRO2 TETR,,,,, SET_REFERENCE_STATE AL2O3 CORUND,,,,, EXPERIMENT HWR=1080:90 </pre> |
| Enthalpy of formation of o-CaZrO ₃ from the component oxides | <pre> CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE ZRO2_MONO HALITE CAZRO3_O=ENT 1 SET_CONDITION T=298.15 P=101325 N(CAO)=.5 SET_CONDITION N(ZRO2)=.5 LNAC(O)=-20 SET_REFERENCE_STATE CAO HALITE,,,, SET_REFERENCE_STATE ZRO2 ZRO2_MONO,,,, EXPERIMENT HMR(CAZRO3_O)=-15960:5% </pre> |

Chemical Potentials via EMF Measurements

You can use chemical potentials and activities/activity coefficients from electromagnetic field (EMF) measurements in the POP-file.

EXAMPLE

| Example | ED_EXP commands |
|----------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Emf data on Cu(s)/Cu ₂ O(s) | <pre> CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC CU2O=FIX 1 CHANGE_STATUS PHASE O2GAS=DORM SET_CONDITION P=101325 T=1000 SET_REFERENCE_STATE O O2GAS,, 100000 EXPERIMENT MUR(O)=-95387:1000 </pre> |

Driving Force for Metastable Phases

You can use chemical driving forces for metastable phases in the POP-file.

EXAMPLES

| Example | ED_EXP commands |
|-----------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| To prevent BCC_A2 to be stable | <pre> CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC_A1 M7C3 M23C6=FIX 1 CHANGE_STATUS PHASE BCC_A2=D SET_CONDITION P=101325 T=1473 EXPERIMENT DGM(BCC)<-0.1:0.1 </pre> |
| To promote CEMENTITE to be stable | <pre> CHANGE_STATUS PHASE BCC M7C3 GRAPHITE=FIX 1 CHANGE_STATUS PHASE CEMENTITE=DORMANT SET_CONDITION P=P0 T=973 EXPERIMENT DGM(CEM)>0.1:0.01 </pre> |

Pressure-Temperature-Volume EOS Data

You can use Pressure-Temperature-Volume Equation of State (EOS) data in the POP-file. Such data includes, for example, molar volume, density, thermal expansion and bulk modulus/compressibility.

| Example | ED_EXP commands |
|---------------------|----------------------------------------------------------------------------------------------------------------------------------------|
| Volume of liquid Pt | <pre> CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE LIQUID=ENT 1 SET_CONDITION P=101325 N=1 T=1873 EXPERIMENT VM=1.00758E-5:5% </pre> |
| Thermal expansion | <pre> CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC_A1=ENT 1 </pre> |

| Example | ED_EXP commands |
|---------|----------------------------------------------------------------------------------------------------------------|
| | <pre>SET_CONDITION P=101325 N=1 T=400 ENTER_SYMBOL FUNCTION ALPHA=VM.T/VM/3; EXPERIMENT ALPHA=2.35E-5:5%</pre> |

Crystal Structure, Lattice Parameters and Site-Occupancy

You use information about defects, ordering or site occupancy, as well as information about crystal structures in the form of lattice parameter values. This information may come from measurements made by X-ray, neutron diffraction, Mössbauer spectroscopy or perturbed angular-correlation.

EXAMPLES

| Example | ED_EXP commands |
|------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Lattice parameter for fcc | <pre>CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC_A1=ENT 1 SET_CONDITION P=101325 N=1 T=298.15 SET_CONDITION X(CR)=0.05 ENTER_SYMBOL FUNCTION LPFCC=((4*VM/6.02214179E23)**(1/3))*1E10; EXPERIMENT LPFCC=4.02:5%</pre> |
| Lattice parameter for bcc | <pre>CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE BCC_A2=ENT 1 SET_CONDITION P=101325 N=1 T=298.15 SET_CONDITION X(AL)=0.08 ENTER_SYMBOL FUNCTION LPBCC=((2*VM/6.02214179E23)**(1/3))*1E10; EXPERIMENT LPBCC=2.90:5%</pre> |
| Site-occupancy, degree of inversion for spinel | <pre>CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE SPINEL=ENT 1 SET_CONDITION P=101325 N(MG)=1 N(AL)=2 N(O)=4 SET_CONDITION T=1073 EXPERIMENT Y(SPINEL,AL+3#1)=0.31:5%</pre> |

Magnetism and Other Atomistic Properties

You can use data about atomistic properties such as magnetism and Curie temperatures in the POP-file.

EXAMPLE

| Example | ED_EXP commands |
|------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Curie temperature of $\text{Mn}_x\text{Fe}_{3-x}\text{O}_4$, $x=1.26$ | <pre>CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE SPINEL=ENT 1 SET_CONDITION T=520 P=101325 N(O)=4 SET_CONDITION N(Fe)+N(Mn)=3 N(Mn)=1.26 EXPERIMENT TC(SPINEL)=520:5</pre> |

Data About Systems of Different Orders

You might want to use data about systems of different orders in the same optimization, such as data about a binary equilibrium with components A and B in a ternary system with components A, B and C, together with data about equilibria in the binary system with components A and B. To do this, you must first suspend all components in the ternary system (A, B and C), and then set the two components you want binary information on (A and B) to status `ENTERED`.

Suspending all components is done by giving the initialization code 0 to the ["CREATE_NEW_EQUILIBRIUM" on page 159](#) command. The components about which you want to use binary information must then be entered again using the ["CHANGE_STATUS" on page 220](#) command.

| Example | ED_EXP commands |
|----------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------|
| A binary (A-B) three-phase equilibrium (FCC-BCC-LIQ) in a ternary system (A-B-C) | <pre>CREATE_NEW_EQUILIBRIUM 1 0 CHANGE_STATUS COMPONENT A B = ENTERED CHANGE_STATUS PHASE FCC BCC LIQ=FIX 1 SET_CONDITION P=1E5 EXPERIMENT T=1177:10</pre> |

Thermodynamic Models

The most common models used in assessments are described briefly in these topics. Examples of how to write the phase definitions in the setup-file are also given for each of these models. In addition to the models described here, a large number of thermodynamic models for various phases in different states have been implemented.

In this section:

| | |
|-----------------------------------------|----|
| Gas | 66 |
| Compound Energy Formalism | 66 |
| Substitutional Liquid | 67 |
| Ionic Two-Sublattice Liquid Model | 67 |
| Models for Ordered Phases | 68 |
| 4SL Model for FCC, HCP and BCC | 69 |
| 2SL Model for FCC, HCP and BCC | 70 |
| Magnetic Ordering | 71 |
| Molar Volumes and High Pressure | 71 |
| Excess Models | 72 |

Gas

The gaseous mixture phase is usually treated as a substitutional phase without sublattice. In the gaseous mixture phase, there are usually molecules formed, and the number of constituents of the gas phase is often much larger than the number of elements. These complex constituents have to be defined as species. The ideal gas model may handle a gas phase under low pressures (and low temperatures). This implies that the P-V-T relations and thermodynamic properties of pure gaseous species are calculated as for ideal gas, and that there is interaction between gaseous species in the mixture. In a defined system, there may only exist one gaseous mixture phase. Type code `G` is used for the gas phase:

```
ENTER_PHASE GAS G, 1 H,H1O1,H1O2,H2,H2O1,H2O2,O,O2,O3; N N
```

Compound Energy Formalism

If the atoms are sufficiently different in size, electronegativity or charge, they may prefer different types of sites in the lattice of crystalline solids. In some cases, a solute atom may even occupy interstitial sites between the normal lattice sites. All such phenomena are treated in Thermo-Calc by the sublattice concept. The Compound Energy Formalism (CEF) has proved to be the most general formalism for many different types of solution phases. It is therefore by default applied to various solid solution phases in the Thermo-Calc software package. CEF can also take ionic constraints (charged cation/anion species) into account. For a comprehensive description on the CEF, please see Hillert (2001), Frisk and Selleby (2001), Sundman and Ågren (1981).

Since the CEF is used by default, no special notation is needed in the phase definition, except for ionic phases, where type code `I` is given.

EXAMPLES

Examples of phase definitions in a setup-file using the CEF:

```
ENTER_PHASE SPINEL I, 4 1 2 2 4
    FE+2,FE+3; FE+2,FE+3,VA; FE+2,VA; O-2; N N
ENTER_PHASE SIGMA, 3 10 4 16
    AL,CO,CR,FE,NB; AL,CO,CR,FE,NB; AL,CO,CR,FE,NB; N N
ENTER_PHASE FCC_A1, 2 1 1
    CR,FE,MN; C,N,VA; N N
ENTER_PHASE BCC_A2, 2 1 3
    CR,FE,MN,VA; C,N,VA; N N
```

Substitutional Liquid

The liquid phase is normally (but not always) modelled as a substitutional phase with no sublattice, which is occupied by two or more constituents. The constituents are normally the elements, but molecules or associates can also be used. Type code `L` is used for the liquid phase.

EXAMPLE

```
ENTER_PHASE LIQUID L, 1
    AL,C,CR,FE,MO,NI,SI ; N N
ENTER_PHASE LIQUID L, 1
    C,FE,FEO,FEO3/2,NI,NIO ; N N
```

Ionic Two-Sublattice Liquid Model

Within the framework of the CEF, the ionic two-sublattice liquid (I2SL) model was developed to be used when there is a tendency for ionization in the liquid, which happens in liquid oxides and sulphides for example. The same model can be used both for metallic and oxide melts. At low levels of oxygen, the model becomes equivalent to a substitutional solution model between metallic atoms. Two sublattices are assumed, one containing charged cations and one containing charged anions, neutrals and vacancies. The complication for an ionic liquid is that the numbers of sites on the cation sublattice and anion sublattice vary with the composition to preserve electroneutrality. For a comprehensive description on the I2SL model, see Hillert et al. (1985), Sundman (1991). In these references, the possible excess parameters are also discussed. Type code `Y` is used for the I2SL model.

EXAMPLE

Examples of phase definitions in a setup-file:

```
ENTER_PHASE LIQUID Y,  
    AL+3,CR+2,FE+2,NI+2; VA; N N  
ENTER_PHASE IONIC_LIQ Y,  
    CA+2,MG+2; O-2; N N  
ENTER_PHASE IONIC_LIQ Y,  
    AL+3,CA+2,FE+2,MG+2,SI+4;  
    ALO2-1,O-2,SIO4-4,VA,FEO3/2,SIO2; N N
```

Models for Ordered Phases

Some solution phases have chemical order-disorder transformations: for example, the disordered FCC_A1 phase can transform to the ordered L1₂ or L1₀ structure where the atoms of different kinds occupy different sublattices. In some cases, it may be advantageous and easy to describe such ordered structures as completely different phases; but in some other cases, like the B2-ordered BCC structure in Al-Fe, the disordered and ordered structures must be described as one single phase because the transformation is of second order along a line in temperature and composition.

The ordering can easily be described by the CEF. For instance, an ordered FCC phase with only L1₂ or L1₀ ordering can be efficiently handled by the so-called Two Substitutional-Sublattice Ordering Model (2SL model), while an ordered FCC with both L1₂ and L1₀ ordering must be described with four sublattices using the so-called Four Substitutional-Sublattice Ordering Model (4SL model). Please note that in both these models, all the substitutional constituents must enter into these sublattices. In addition, you may also have one sublattice for interstitials.

Thermo-Calc supports a feature of splitting the parameters of a chemically ordered phase onto two different phase descriptions. This is very convenient. In this way, you can have one phase for all parameters describing the disordered state (the configuration independent state) and in the other phase only those parameters needed to describe the remaining part (the configuration dependent part), that is, the Gibbs energy contribution due to the ordering transformation. This has been implemented in such a way that the contribution from the configuration dependent part is zero when the solution phase is disordered. The optimization of the disordered phase is independent of the order-disorder transformation; the ordering energy is an add-on to the disordered part. This is particularly useful in higher order systems, as an ordered phase can dissolve several elements that have no particular contribution to the actual ordering. The phases Gibbs energy add together by giving this command in the setup-file: `AMEND_PHASE_DESCRIPTION <ordered phase> disordered_part <disordered phase>`

Since PARROT does not automatically create new composition sets, it is necessary to create composition sets for both the ordered and disordered phases in the setup-file: Amend_
phase_description <phase> composition_sets <new highest set number>,,, ,

EXAMPLE

Example of phase definitions for the corresponding disordered and ordered parts in a setup-file:

```
ENTER_PHASE FCC_A1, 2 1 1
      AL,CR,FE,NI; VA; N N
ENTER_PHASE FCC_L12, 3 .75 .25 1
      AL,CR,FE,NI ; AL,CR,FE,NI; VA; N N
AMEND_PHASE_DESCRIPTION FCC_L12 DIS_PART FCC_A1
```

4SL Model for FCC, HCP and BCC

Ordered FCC, HCP and BCC solution phases handled by the 4SL model requires four sublattices for substitutional ordering and can additionally have an interstitial sublattice. A 4SL model is especially useful for modelling different kinds of ordered phases that are based on the same disordered phase, such as L1₀ and L1₂ based on FCC_A1, and B2, D0₃, L2₁ and B32 based on BCC_A2 etc.

For ordered FCC or HCP phases, these four substitutional sublattices represent four corners of the regular tetrahedron on these lattices, all of which are the nearest neighbours. These corners are equivalent lattice points, thus all G parameters for each end-member with the same elements, but distributed on different sites, must be identical. It should be emphasized that the end-member energy here represents the ordering energy rather than the formation energy of the compound.

The constraints on the parameters in the 4SL model can be derived based on the symmetry of the lattice:

$$G_{A:B:B:B}=G_{B:A:B:B}=G_{B:B:A:B}=G_{B:B:B:A}$$

$$G_{A:A:B:B}=G_{A:B:A:B}=G_{A:B:B:A}=G_{B:A:A:B}=G_{B:A:B:A}=G_{B:B:A:A}$$

$$G_{B:A:A:A}=G_{A:B:A:A}=G_{A:A:B:A}=G_{A:A:A:B}$$

$$L_{A,B:*.:.}=L_{*:A,B:*.}=L_{*:*.A,B:}=L_{*:*.:.A,B}$$

The asterisk * means that the interaction parameter is independent of the occupation of that sublattice. For the disordered phase to be completely disordered, i.e. that all site fractions are equal on all four sublattices, all constraints must be correct.

For ordered BCC phases, the situation is a bit more complicated, as the four sublattice ordering phase represents an irregular tetrahedron with two pairs of sites that are next nearest neighbours. Thus, for an A-B binary solution phase, with A located on two sublattice sites and B on the other two, the end-member described by $G_{A:A:B:B}$ has four nearest neighbour bonds between A and B atoms, whereas the end-member described by $G_{A:B:A:B}$ has two nearest neighbour bonds between A and B atoms and two next nearest neighbour bonds. Many parameters thus have a relation:

$$G_{A:B:B:B}=G_{B:A:B:B}=G_{B:B:A:B}=G_{B:B:B:A}$$

$$G_{B:A:A:A}=G_{A:B:A:A}=G_{A:A:B:A}=G_{A:A:A:B}$$

$$G_{A:A:B:B}=G_{B:B:A:A}$$

$$G_{A:B:A:B}=G_{A:B:B:A}=G_{B:A:A:B}=G_{B:A:B:A}$$

$$L_{A,B:*.:.}=L_{*.A,B:*.}=L_{*.:.A,B:*=L_{*.:.*.A,B}$$

The $G_{A:B:B:B}$ term represents DO_3 , $G_{A:A:B:B}$ B2 and the $G_{A:B:A:B}$ B32 ordering. There are also two kinds of reciprocal interaction parameters:

$$L_{A,B:A,B:*.:.};0...9$$

$$L_{A,B:*.A,B:*.};0...9$$

Kusoffsky et al. (2001) have shown the influence of different parameters available in the 4SL model applied to fcc ordering. The possibility to use the 4SL model to BCC ordering has been studied by Sundman et al. (2009) in the Al-Fe system.

2SL Model for FCC, HCP and BCC

The reason for using a 2SL model instead of a 4SL model is that the calculations are faster, but on the other hand it can only model one kind of ordered phase(s). For instance, it is not possible to model FCC with both $L1_0$ and $L2_1$, or BCC with DO_3 and B2, etc.

In order to get the fully disordered phase to form, constraints are needed as for the 4SL model. For the symmetric phases, e.g. B2 and $L1_0$, the relation between parameters are:

$$G_{A:B}=G_{B:A}$$

$$L_{A,B:*=L_{*.A,B}$$

For a 2SL asymmetric model including, but not limited to, $L1_2$, more constraints are needed. This model has many complicated relations between the parameters. The relation between the parameters for the 2SL $L1_2$ model can be derived from a 4SL model. The conversion from 4SL model parameters to 2SL parameters for $L1_2$ can be found in Dupin et al. (2001) and for $L1_0$ in Yuan et al. (2012). Higher-order systems with an $L1_2$ phase modelled with two

sublattices require a lot of ternary and some quaternary interaction parameters in order to make the disordered state stable. These parameters have been derived by e.g. Dupin (1995), also found in Kusoffsky et al. (2001).

Many publications exist on how to model order/disorder transformations using a two-sublattice model, see e.g. Dupin, Ansara (1999), De Keyser et al. (2009).

Magnetic Ordering

The magnetic contribution to the Gibbs energy is given by a model proposed by Inden (1975) and adapted by Hillert and Jarl (1978), and is described by:

$$G = RT \ln(b+1) f(t)$$

where $t = T/T_C$.

The values of the Curie temperature, T_C , and Bohr magneton number, b , at a certain composition are then used in an optimization procedure to calculate the contribution to Gibbs energy due to magnetic ordering. Curie temperature and Bohr magneton number are given in the command ["ENTER_PARAMETER" on page 268](#) for phases that undergo a magnetic transition:

```
AMEND_PHASE_DESCRIPTION BCC_A2 MAGNETIC -1.0 0.4
ENTER_PARAMETER TC(BCC_A2,FE:VA;0) 298.15 +V1; 6000 N
ENTER_PARAMETER BMAGN(BCC_A2,FE:VA;0) 298.15 +V2; 6000 N
```

The arguments -1 and 0.4 specify the values of parameters in the magnetic model: -1 is the antiferromagnetic factor and 0.4 is the structure factor. Usually the antiferromagnetic factor = -1 for bcc and = -3 for fcc (and other non-bcc phases). The structure factor corresponds to the short range order fraction of the enthalpy. This factor is 0.4 for bcc and 0.28 for non-bcc phases.

Molar Volumes and High Pressure

Including volumes in a thermodynamic database enable calculations of volume changes, volume fraction, lattice mismatch in cubic structures and phase diagrams at increased pressure. Pressure independent volumes can be used up to about 1 GPa. At pressures above 1 GPa the pressure dependence of the volumes must be included by using a proper equation of state (EOS). An EOS has been developed by Lu et al. (2005), based on the EOS from Jacobs and Oonk (2000). Four parameters are used in the implementation of the model in ThermoCalc:

- v_0 : Volume at 1 bar and at reference temperature T_0
- v_A : Integrated thermal expansivity

- VK: Isothermal compressibility at 1 bar
- VC: Parameter to fit high pressure data

All parameters can be composition dependent in the same way as all other model parameters in Thermo-Calc. Experimental information about the temperature, pressure and composition dependence of the volume can be assessed using these model parameters. To evaluate V0, VA and VK experimental data at 1 bar only are needed.

EXAMPLE

Examples on modelling molar volume in a setup-file:

```
ENTER_PARAMETER V0 (BCC_A2, FE:VA;0) 298.15 +V1; 6000 N
ENTER_PARAMETER VA (BCC_A2, FE:VA;0) 298.15 +V2*T+V3*T**2; 6000 N
ENTER_PARAMETER VC (BCC_A2, FE:VA;0) 298.15 +V4+V5*T; 6000 N
ENTER_PARAMETER VK (BCC_A2, FE:VA;0) 298.15 +V6+V7*T; 6000 N
ENTER_PARAMETER V0 (FCC_A1, CR, FE:VA;0) 298.15 +V8; 6000 N
ENTER_PARAMETER VA (FCC_A1, CR, FE:VA;0) 298.15 +V9*(T-298.15); 6000
N
```

Excess Models

Unless specifically amended, the excess Gibbs energy terms are modelled by the Redlich-Kister-Muggianu Model. Other excess models for the Gibbs energy are also implemented in Thermo-Calc, such as e.g. Kohler and Toop-Kohler extrapolation models.

Thermo-Calc is not restricted to binary interaction parameters. Ternary, quaternary and higher-order interaction parameters can also be used if there is enough information to evaluate these from experimental data. The ternary interaction parameters are identified by the degrees of the so-called ternary L parameter (i.e. 0, 1 and 2) in the command ["ENTER_PARAMETER" on page 268](#). If the parameter is composition-independent, you only need a single interaction parameter with a degree of zero, i.e. only the ⁰L term. If there is a ternary composition-dependent interaction parameter, you must enter all three parameters (0,1 and 2). If such a ternary interaction parameter should be zero, then assign it a function which is zero. If the three interaction parameters have the same value, then that is identical to having a composition-independent ternary parameter.

EXAMPLE

```
ENTER_PARAMETER L (LIQUID, A, B, C;0) 298.15 +1000; 6000 N
ENTER_PARAMETER L (LIQUID, A, B, C;1) 298.15 +1000; 6000 N
```

```
ENTER_PARAMETER L(LIQUID,A,B,C;2) 298.15 +1000; 6000 N
```

is identical to

```
ENTER_PARAMETER L(LIQUID,A,B,C;0) 298.15 +1000; 6000 N
```

This also means that

```
ENTER_PARAMETER L(LIQUID,A,B,C;0) 298.15 +1000; 6000 N
```

```
ENTER_PARAMETER L(LIQUID,A,B,C;1) 298.15 +ZERO#; 6000 N
```

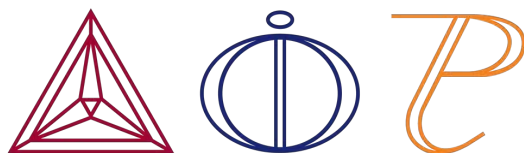
```
ENTER_PARAMETER L(LIQUID,A,B,C;2) 298.15 +ZERO#; 6000 N
```

is NOT identical to

```
ENTER_PARAMETER L(LIQUID,A,B,C;0) 298.15 +1000; 6000 N
```

Database Manager User Guide

Thermo-Calc Version 2020a



Introduction to the Database Manager Guide

In this section:

| | |
|----------------------------------------------------|---|
| Thermodynamic and Kinetic/Mobility Databases | 3 |
| Initialization of the TDB Module | 3 |

Thermodynamic and Kinetic/Mobility Databases

This guide describes how to define and construct a thermodynamic or kinetic database. It includes details about the data structures and formats of the Thermo-Calc databases as well as the Diffusion Module (DICTRA) database-extensions.

The Thermo-Calc databases are created and maintained in the Thermo-Calc Database Format (TDB) which is an international standard for the CALPHAD-type thermodynamic calculations and kinetic simulations. This document gives a full description of the TDB format (with the Diffusion Module (DICTRA) database extension) and is a comprehensive guide about how to create and manage a Thermo-Calc (and Diffusion Module (DICTRA)) database.

Usually, a Thermo-Calc or Diffusion Module (DICTRA) database is constructed as a single text file with an extension of TDB, for example, `PAQ2setup.TDB`. For some databases (especially large databases used with older versions of Thermo-Calc or Diffusion Module (DICTRA)) a database may consist of one primary-definition file (`***setup.TDB`) and several additional-definition TDB files (such as `***param.TDB`, `***funct.TDB`, `***refer.TDB`, etc. These are built for a variety of defined parameters, functions, references and so forth, and are linked to the `***setup.TDB` file through the correct use of the ["TYPE_DEFINITION"](#) on [page 19](#) and/or ["FTP_FILE"](#) on [page 22](#) commands inside the `***setup.TDB` file.



With Thermo-Calc, Precipitation Module (TC-PRISMA) and Thermo-Calc Software Development Kits (SDKs), you can code everything into a single `***setup.TDB` file for a database at any scale.

Initialization of the TDB Module

The following explains how a database initialization file is constructed to work with the so-called TDB (database) module. When you start, the TDB module looks for a file that has information about the available standard databases. The database initialization file is called `tc_initd.tdb`. By default it is located in the `data` subdirectory of the Thermo-Calc installation directory.



See ["Database Installation Folder" on page 32](#) in the *Thermo-Calc User Guide*.

The location can be overridden by:

- A command line parameter `-t` followed by the path to the directory containing the `tc_initd.tdb` file.
- The environment variable `TC_DATABASE_DIRECTORY` pointing to the directory containing the `tc_initd.tdb` file. This overrides both the default value and a directory given with the `-t` command line argument.

Each database defined in `tc_initd.tdb` represents a database that can be used within Thermo-Calc. Each entry has three parts:

- the database short-name (e.g. `FEDEMO`, maximum seven characters),
- the path to the database setup file (max 78 characters), and
- a short description of the database (max 60 characters). The entry must end with an exclamation mark (!), the first two parts must not contain white space, and it can span over two lines.

The paths can be relative to the `tc_initd.tdb` file or absolute. For platform independence, the recommendation is to always use forward slashes (/) in the paths, but on Windows backslash (\) also works.

You can add comment lines in the database initialization file. Comments must start with a `$` sign.



Each entry record (i.e. for a single database) must finish with an exclamation mark !. There should be no spaces or commas within the first and second fields since these characters are taken as field separators, while spaces or commas can be used in the third field.

EXAMPLE OF AN INITIALIZATION FILE

The following are examples of an initialization file defining two databases:

```
SSOL7 SSOL7\SSOL7SETUP.TDC  SGTE Solutions Database version 7.0 !
MYDB1 ../../../../MYDATABASES/ABC.TDB My database 1.0 !
```

The Database Definition File and Keywords

In this section:

| | |
|---------------------------------------|----|
| Database Definition File Syntax | 6 |
| ELEMENT | 7 |
| SPECIES | 8 |
| PHASE | 9 |
| CONSTITUENT | 14 |
| ADD_CONSTITUENT | 15 |
| COMPOUND_PHASE | 16 |
| ALLOTROPIC_PHASE | 16 |
| TEMPERATURE_LIMITS | 17 |
| DEFINE_SYSTEM_DEFAULT | 17 |
| DEFAULT_COMMAND | 17 |
| DATABASE_INFORMATION | 18 |
| TYPE_DEFINITION | 19 |
| FTP_FILE | 22 |
| FUNCTION | 23 |
| PARAMETER | 26 |
| OPTIONS | 33 |
| TABLE | 34 |
| ASSESSED_SYSTEMS | 35 |
| REFERENCE_FILE | 38 |
| LIST_OF_REFERENCE | 39 |
| ADD_REFERENCE | 40 |
| CASE and ENDCASE | 41 |
| VERSION_DATA | 42 |

Database Definition File Syntax

The database definition (*.TDB) file (normally named `***setup.TDB`) consists of a set of keyword codes each followed by one or several parameters (arguments).

- A complete keyword entry must end with an exclamation mark (!).
- A single keyword entry can be up to 2000 characters long. However, the maximum length of a line in an *.TDB file is 78 characters--it may be necessary to continue the keyword parameter (arguments) on several lines. The ! must be at the end of the last line.
- It is recommended to always have at least one empty space at the beginning of each continuation line for the keyword parameters (arguments); otherwise, the DATA module can misunderstand the parameters (or arguments), or issue an error message.
- The keyword and its various parameters (arguments) are separated by a space or a comma.
- A dollar sign (\$) in the first position of the line indicates that the line is a comment line, which is ignored by the DATA module.

When the database is selected the DATA module only reads the database definition file (`***setup.TDB`) once, from beginning to end. The DATA module checks continuously when reading the definition file. This implies that (nearly) everything must be declared or defined before it is used in any other way.

For example, if the GRAPHITE phase is to be included in the database definition, the element C (carbon) and the phase GRAPHITE must be defined before declaring that carbon dissolves in graphite. This definition order is necessary to build the internal data structure acceptable by the DATA module (during its consistency checking).

This topic gives a description of the available keywords and the appropriate arguments. A basic knowledge of the Gibbs Energy System (GIBBS) module is assumed.

This syntax is used:

```
KEYWORD [arg.1]*# [arg.2]*## {optional arg.3}!
```

The keywords are written in full length but can be abbreviated as long as the abbreviation is unique. A keyword may have syntax consisting of several arguments and optional arguments. The number, # or ##, in the notation, [...] *# or [...] *##, indicates an argument with a maximum length of # ASCII characters.



Arguments within square brackets [...] must always be given, but are optional when enclosed in curly brackets {...}.

ELEMENT

```
ELEMENT [element name]*2 [ref. state]*24 [mass] [H298] [S298] !
```

The *element name* (maximum two characters) is the one found in the periodic chart but there are no naming restrictions. However, the GIBBS module only recognizes UPPER-case element names (if the `Upper Case Mode` is selected by the GIBBS command ["REINITIATE" on page 242](#)), which means that lower-case (if defined in a database) is automatically converted to UPPER-case by the DATA/GIBBS module.

The elements are automatically entered as species using the same names of the elements. If, for example, the species corresponding to FE needs to be named FE1, you can define the species as FE1, which results in an element named FE and a species named FE1. Vacancies (VA) and electrons (denoted either as /- in gaseous, liquid or solid phases, or ZE in an aqueous solution phase), need to be entered as special elements for correct handling by the DATA module.

The *reference (ref.) state* (maximum 24 characters) is the stable phase (at 298.15 K and 1 bar) that should contain this element and be used as the reference state for all element thermodynamic data. The *mass*, given in gram per mole, is used in various calculation programs and should always be given the correct value. *H298* and *S298* denote the enthalpy and entropy difference between 0 and 298.15 K for the element in SI units. If these are unknown, the values can be set to zero. All this information (reference state, H298 and S298) define the SER (Stable Element Reference state).

EXAMPLES

```
ELEMENT /- ELECTRON_GAS      0.0  0.0  0.0 !
ELEMENT VA VACUUM            0.0  0.0  0.0 !
ELEMENT ZE UNIT_CHARGE       0.0000000001  0.0  0.0 !
ELEMENT AL FCC_A1            26.98154 4577.296 28.3215 !
ELEMENT C GRAPHITE           12.011  1054.0   5.74 !
ELEMENT FE BCC_A2            55.847  4489    27.28 !
ELEMENT O 1/2_MOLE_O2 (G)    15.9994 4341    102.5158 !
ELEMENT TI HCP_A3            47.88   4810    30.648 !
ELEMENT ZR HCP_A3            91.224  5566.27  39.181 !
```

SPECIES

```
SPECIES [species name]*24 [stoichiometric formula] !
```

This keyword defines species in the data structure. Every *species name* (maximum 24 characters) must be unique. The species are built from the predefined set of elements in the stoichiometric formula. If an undefined element is referenced, DATA displays an error message and the data structure is probably damaged.

The species names do not have to be the same as the stoichiometry formula, although in general this is recommended. The elements are automatically entered as species using the same names of the elements.



You can define a species name as a mixture of UPPER-case and lower-case letters in a database, but the DATA module automatically converts all lower-case to UPPER-case because the GIBBS module only recognizes UPPER-case species names.

When naming the species in a database, use special characters (such as +, -, _, / and .) in species names. Avoid using other special characters (such as (and)).

The *stoichiometric formula* is written with a simplified chemical notation, in which the chemical elements should always be given in UPPER-case and in any preferred order, and the stoichiometric coefficients are written in either real numerical factors or integer digits.



It is important that the numerical factor of 1 is not left out. Subgroups are not allowed in a stoichiometry formula; however, while specifying the stoichiometry formula for a specific species in a database, you can specify it in a way that some elements (always together with the corresponding partial stoichiometric coefficients) are repeated (as in the examples below).

EXAMPLES

```
SPECIES AL2O3      AL2O3 !
SPECIES Silica     SI1O2 !
SPECIES NaSb_6OH   NA1SB1O6H6 !
SPECIES FE+2       FE/+2 !
SPECIES SB-3       SB/-3 !
```

```

SPECIES AlCl2/3          AL.33333CL.666667 !
SPECIES Al1CL1H2O2      AL1CL1H2O2 !
SPECIES AlCl3_3H2O      AL1CL3H6O3 !
SPECIES AlO2H2Cl.H6O3   AL1O2H2CL1H6O3 !
SPECIES AlCl2-OH.3H2O    AL1CL2O1H1H6O3 !
SPECIES AlCl2OH.3Water   AL1O1H1CL2H6O3 !

```

PHASE

```

PHASE [phase name]*24 [data-type code]*8 [numb. subl.] [sites in
subl. 1] [sites in subl. 2] etc... {auxiliary text string} !

```

This keyword defines a phase and its properties (except for what species are allowed to enter it and for its parameters).

The *phase name* (maximum 24 characters) must be unique; otherwise the DATA module sees it as an attempt to redefine a previously defined phase. This causes DATA to display an error message and ignore the rest of the line. A phase name can be suffixed by an underscore (_) and letters to identify the physical state(s) or structure type(s) of the phase.

Examples of Recommended Suffixes

| Suffix | Definition |
|---------|----------------------------------------------------|
| ABC_S | The ABC phase in solid state. |
| ABC_S2 | The ABC phase in solid state 2. |
| ABC_S3 | The ABC phase in solid state 3. |
| ABC_LT | The ABC phase in solid state at low temperatures. |
| ABC_HT | The ABC phase in solid state at high temperatures. |
| ABC_L | The ABC phase in liquid state. |
| ABC_LIQ | The ABC phase in liquid state. |
| FCC_A1 | The FCC phase in disordered structure type A1. |
| FCC_L12 | The FCC phase in ordered structure type L12. |

The *phase name* can also be attached with a colon sign (:) and a letter for a legal GIBBS phase-type code (e.g. IONIC_LIQ:Y and GAS:G).

GIBBS Phase-type Codes

| Code | Definition |
|------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| G | Bit set for a gaseous mixture phase. |
| A | Bit set for an aqueous solution phase. |
| Y | Bit set for an ionic liquid solution phase (specially treated by the Ionic Two-Sublattice Liquid Model). |
| L | Bit set for a liquid solution phase (but not A (aqueous) or Y (ionic liquid)). |
| I | Bit set for a phase with charged species (but not G (gaseous), A (aqueous) or Y (ionic liquid)). |
| F | Bit set for an ordered FCC or HCP solution phase using the <i>Four Substitutional-Sublattice Ordering Model</i> (additionally, such a phase can also have interstitial sublattices). |
| B | Bit set for an ordered BCC solution phase using the <i>Four Substitutional-Sublattice Ordering Model</i> (additionally, such a phase can also have interstitial sublattices). |



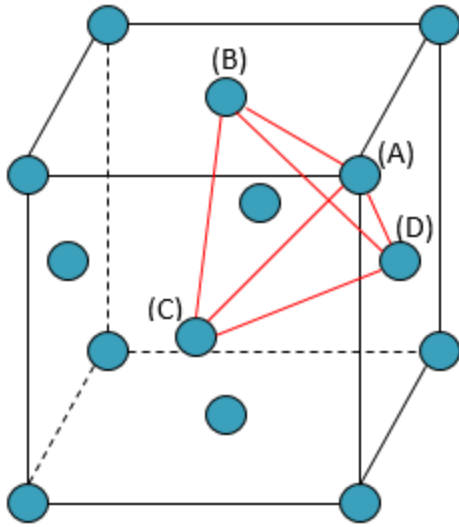
Other invalid characters (e.g. \mathbb{M} or \mathbb{P}) are eventually treated, together with the colon (:) as a part of a phase name.

A \mathbb{G} phase (gaseous mixture) or an \mathbb{A} phase (aqueous solution) is usually treated as a substitutional phase without sublattice, and an \mathbb{L} phase (ordinary liquid solution) is normally (but not always) modelled as a substitutional phase without sublattice, too.

For ordered FCC or HCP phases, these four substitutional sublattices represent four corners of the regular tetrahedron on these lattices, all of which are the nearest neighbours, as shown.

FCC UNIT CELL EXAMPLE

An FCC unit cell with the lattice positions indicated that correspond to the \mathbb{G} (FCC,A:B:C:D) end member. All lattice positions are equivalent for a four substitutional-sublattice ordering model.



A *Normal 4-Sublattice Model* requires that all the G parameters for each of the end-members with the same elements but distributed on different sites be given separately. However, as these corners are identical lattice points, the phase-type option F means that the G parameters need be given only once. The possible permutations are handled automatically.

Additional clarification

An $A-B$ binary solution phase (with the element A located on one sublattice site and B on the other three sublattice sites) treated by the Normal 4-Sublattice Model has to have four G parameters for four end-members, i.e.

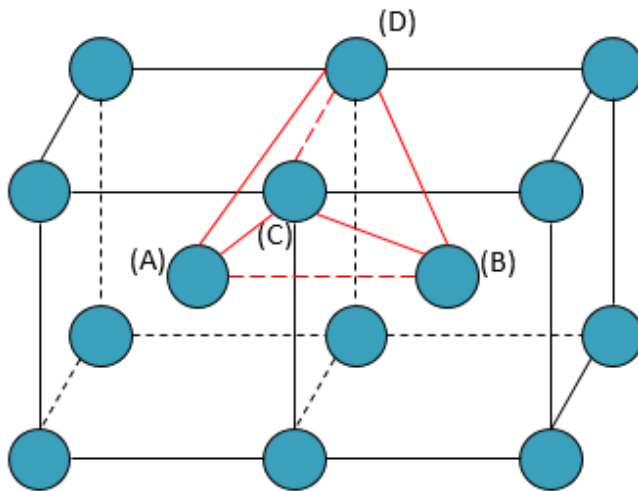
- $G(\text{phase}, A:B:B:B)$
- $G(\text{phase}, B:A:B:B)$
- $G(\text{phase}, B:B:A:B, \text{ and}$
- $G(\text{phase}, B:B:B:A)$

This is because in the general case these G parameters can be different from each other. But for the FCC and HCP orderings, they are identical and thus all G parameters of such end-members need to be given only once, and the possible permutations are then automatically handled by the GIBBS module. Also, only one of the identical permutations is listed; in this example, $G(\text{phase}, A:B:B:B)$ where it is alphabetically the first in the list of permutations. This significantly simplifies the usage of this model (*Four Substitutional-Sublattice Ordering Model*) in multicomponent alloys.

For ordered BCC phases, the phase-type option B means the same thing but it is more complicated since the 4-substitutional-sublattice ordering phase represents an irregular tetrahedron with two pairs of sites that are next nearest neighbours as shown:

BCC UNIT CELL EXAMPLE

Two BCC unit cells with the lattice positions indicated that correspond to the $G(\text{phase}, A:B:C:D, 0)$ end member. Lattice positions (A) and (B) are equivalent, as are lattice positions (C) and (D) for a four substitutional-sublattice ordering model.



For an end member described by the parameter $G(\text{phase}, A:B:C:D)$ A and B are next nearest neighbours, as are C and D. And the nearest neighbours of A (or B) are C and D. Thus, for an $A-B$ binary solution phase (with the element A located on two sublattice sites and B on two sublattice sites) treated by the Normal 4-Sublattice Model, the end-member described by the $G(\text{phase}, A:A:B:B)$ term has four nearest neighbour bonds between A and B atoms, whereas the end-member described by the $G(\text{phase}, A:B:A:B)$ term has two nearest neighbour bonds between A and B atoms and three next nearest neighbour bonds.

The first end-member (described by the $G(\text{phase}, A:A:B:B)$ term) represents B2-ordering and the second (described by the $G(\text{phase}, A:B:A:B)$ term) stands for B32-ordering. There are two permutations of the $G(\text{phase}, A:A:B:B)$ term and four permutations of the $G(\text{phase}, A:B:A:B)$ term, automatically conducted in the *Four Substitutional-Sublattice Ordering Model*. If you enter the unary, binary, ternary and quaternary parameters you are dealing with 1, 6, 21, 55 parameters for BCC:B, 1, 5, 15, 35 parameters for FCC:F and 1, 16, 81, 256 parameters for phases without F/B.

An additional feature with the phase-type options **F** and **B** is that a composition set that represents the solution phase has a suffix (indicating what ordering the phase has) that is automatically added to its phase name in some listings of equilibrium calculations (when performing either single-point or stepping or mapping calculations, and when plotting the calculated property diagrams or phase diagrams).

Such suffix indications can be:

| Solution Phase | Suffix for Disordered Phase | Suffix for Ordered Phase |
|----------------|-----------------------------|--------------------------|
| FCC PHASE | FCC_A1 | FCC_L12 |
| | | FCC_L10 |
| BCC PHASE | BCC_A2 | BCC_B2 |
| | | BCC_B32 |
| | | BCC_D03 |
| | | BCC_L21 |
| HCP PHASE | HCP_A3 | HCP_D019 |
| | | HCP_B19 |



If you want to convert an existing database TDB file to use the F/B feature, add the phase-type code to the corresponding phase name in the PHASE and CONSTITUENT commands in the TDB-file, then when running the LIST_DATA command in the Gibbs (GES) module. The created database file is in this less verbose format.

The *data-type code* consists of 1 to 8 characters where each character must stand for an action, which is to be coupled to this phase. The keyword TYPE_DEFINITION, described below, must be used in the current database to specify what action should be taken by DATA for each character code.

The data entries [numb. subl.] [sites in subl. 1] [sites in subl. 2] etc., specify the total number of sublattices (always as an integer digit) and the sites (i.e. stoichiometric coefficients) of each of the sublattices (given in either integer digits or real numerical factors) for the phase.

Optionally, an *auxiliary text string* (maximum 78 characters) can be given after the last [sites in sublattice #] but before the exclamation mark !. This string displays in connection with the phase name in some listings within the DATA module.

EXAMPLES

```

PHASE GAS:G % 1 1.0 !
PHASE LIQUID:L %ZCDQ 2 1.0 1.0
> Metallic liquid solution, modelled by CEF Model. !
PHASE IONIC-LIQ:Y %ZCDQ 2 1.0 1.0
> Ionic liquid solution, modelled by Ionic Two-Sublattice Model. !
PHASE SPINEL:I %ZA 4 1 2 2 4
> Complex Spinel Solution, by CEF model with ionic constraints. !
PHASE M23C6 % 3 20.0 3.0 6.0 !
PHASE FCC_A1 %&A 2 1 1
> Disordered FCC phase; also as MX carbides/nitrides. !
PHASE FCC_L10 %&AX 3 0.75 0.25 1
> Ordered FCC phase, modelled by 2-Sublattice Model for Ordering.
!
PHASE FCC_L12:F %&AX 5 0.25 0.25 0.25 0.25 1.0
> Ordered FCC phase, modelled by 4-Sublattice Model for Ordering.
!
PHASE AQUEOUS:A %HIJMR 1 1.0
> Aqueous Solution: using the Complete Revised HKF Model. !

```

CONSTITUENT

```
CONSTITUENT [phase name]*24 [constituent description]*2000 !
```

This keyword (and the ["ADD_CONSTITUENT" on the next page](#) keyword for large solution phase) defines the phase-constitution as a list of constituents (for a substitutional phase with no sublattice) or of constituent arrays (for a sublattice phase).

The *phase name* (maximum 24 characters) must be a predefined phase (i.e. already through the ["PHASE" on page 9](#) keyword).



It is important that if a phase bears a legal phase-type (among G, A, Y, L, I, F and B) in its phase definition (already by the PHASE keyword; such as GAS:G, SLAG:L, LIQUID:L, IONIC_LIQ:Y, SPINEL:I, FCC_L12:F, HCP_D021:F, BCC_B2:B, AQUEOUS:A), such a valid phase-type code must also always be attached to the phase name in the CONSTITUENT keyword (and the ADD_CONSTITUENT keyword).



Specifying the phase name in UPPER-case is recommended. You can define a phase name as a mixture of UPPER-case and lower-case letters in a database, but the DATA module automatically converts all lower-case to UPPER-case because the GIBBS module only recognizes UPPER-case phase names.

The *constituent description* (maximum 2000 characters) is a list of the species that enter a phase. The list starts with a colon (:), indicating the start of the sub-list of species for the first sublattice, and different sublattices are separated by colons. The complete sequence ends with a final colon.

Optionally, each sublattice may specify which species are considered to be major constituents. This is done by adding a percent sign (%) directly to the species name. The start values on the site fractions of the major constituents should sum to 0.99 on a specific sublattice. Thus, the minor constituents (i.e. those without a %) add up to 0.01. A maximum of 2000 characters can be coded in the constituent description, continuing in sequent lines. If the phase has a constituent description longer than 2000 characters, the rest can be coded in one or several ADD_CONSTITUENT keywords.

EXAMPLES

```

CONSTITUENT BCC_A2 :FE
CONSTITUENT IONIC-LIQ:Y :FE+2 : SB-3: !
CONSTITUENT M23C6 :CR FE :FE CR W MO : C: !
CONSTITUENT AQUEOUS:A :H2O% AG+1 AGF AGCL AGCL2-1 AGI3-2 AGSO4-1
AGC2H4+1
    AGN2H6+1 AGC2N2-1 AGC2H4NO2 AL+3 ALF3 ALO2-1, ... : !
CONSTITUENT SPINEL:I : AL+3% CR+3 FE+2% FE+3 MG+2% NI+2
                        : AL+3% CA+2 CR+3 FE+2 FE+3 MG+2% NI+2 VA
                        : FE+2 MG+2 VA%
                        : N-3 O-2% :!
```

ADD_CONSTITUENT

```
ADD_CONSTITUENT [phase name]*24 [constituent description]*2000 !
```

This keyword adds more constituents to a phase that already has some constituents. Its syntax is the same as for the ["CONSTITUENT" on the previous page](#) keyword. This keyword can be used several times, if the phase is very large, e.g. a gaseous mixture or a complex aqueous solution. This is useful when there are so many constituents in a phase that the 2000 characters available for the constituent description list is not enough.



Constituents are not necessary on all sublattices. In the second example below, no addition is made to the first sublattice.

EXAMPLES

```
ADD_CONSTITUENT GAS :S1 S2 S3 ... : !
ADD_CONSTITUENT IM-PHASE : :CR:W ... : !
ADD_CONSTITUENT AQUEOUS:A :CUCL+1 CUCL2 CUCL2-1 CUCL3-2 CUOH+1
CUO2H2 CUO3H3-1
      CUO4H4-2 CU2OH+3 CU2O2H2+2 CU3O4H4+2 NIO2H2 NIO3H3-1 NIO4H4-2
NI2OH+3
      NI4O4H4+4 ZNOH+1 ZNO2H2 ZNO3H3-1 ZNO4H4-2 ... : !
```

COMPOUND_PHASE

```
COMPOUND_PHASE [phase name]*24 [data-type code]*8 [constituent] !
```

The keyword is a compact way to simultaneously define a species, a *compound phase* (maximum 24 characters) and its phase-constituent. It is useful for stoichiometric phases with constant compositions. The species name and stoichiometric formula must be identical, i.e. being the given *constituent*. The phase has this species as its only constituent. This keyword allows the database definition file for a large substance database to be more compact; it is a combination of the ["SPECIES" on page 8](#), ["PHASE" on page 9](#) and ["CONSTITUENT" on page 14](#) keywords.

EXAMPLES

```
COMPOUND_PHASE AL2O3 % AL2O3 !
COMPOUND_PHASE MAGNETITE %MF FE3O4 !
COMPOUND_PHASE QUARTZ % SIO2 !
```

ALLOTROPIC_PHASE

```
ALLOTROPIC_PHASE [phase name]*24 [data-type code]*8 [constituent]
!
```

This keyword does the same as the ["COMPOUND_PHASE" above](#) keyword for entering an allotropic phase (maximum 24 characters), but does not enter the constituent as a species to the data structure. Use this if the species is already defined.

EXAMPLES

```
ALLOTROPIC_PHASE BETHA-AL2O3 % AL2O3 !
```

```
ALLOTROPIC_PHASE CRISTOBALITE % SIO2 !
ALLOTROPIC_PHASE TRIDYMITE % SIO2 !
```

TEMPERATURE_LIMITS

```
TEMPERATURE_LIMITS [lower limit] [upper limit] !
```

This keyword sets the default upper and lower temperature limits used by the GIBBS module for Gibbs energy parameters and functions. It can be used only once in one database definition file and all its sequential files.

EXAMPLE

```
TEMPERATURE_LIMITS 500.0 1800.0 !
```

DEFINE_SYSTEM_DEFAULT

```
DEFINE_SYSTEM_DEFAULT [keyword] {G-ref. type index} !
```

This keyword sets the default value to ELEMENT or SPECIES in the DATA command ["DEFINE_SYSTEM" on page 125](#).

For a substance database, it can be appropriate to have ELEMENT as a default value whereas a large solution database can benefit from having SPECIES as a default value. A proper default value is useful for beginners. An advanced user is more likely to use the DATA commands DEFINE_ELEMENT and DEFINE_SPECIES to override the default value.

{G-ref. type index} is an integer indicating the reference state type for an element when entering and listing data in the GIBBS module. The following lists legal numbers and the corresponding meaning (the reference state type for an element):

| Number | Definition |
|--------|--------------|
| 1 | symbol: G |
| 2 | symbol: H298 |
| 3 | symbol: H0 |

EXAMPLE

```
DEFINE_SYSTEM_DEFAULT element 2 !
```

DEFAULT_COMMAND

```
DEFAULT_COMMAND [secondary keyword and parameters] !
```

This keyword specifies commands to be executed by the DATA module at database initialization. The syntax of the available command is currently not the same as the user available DATA commands but the actions are similar. The available *secondary keyword and parameters* in syntax are:

```
DEFINE_SYSTEM_ELEMENT [element names]
DEFINE_SYSTEM_SPECIES [species names]
DEFINE_SYSTEM_CONSTITUENT [phase] [sublattice] [species]
REJECT_SYSTEM_ELEMENT [element names]
REJECT_SYSTEM_SPECIES [species names]
REJECT_SYSTEM_CONSTITUENT [phase] [sublattice] [species]
REJECT_PHASE [phase names]
RESTORE_PHASE [phase names]
```

EXAMPLES

```
DEFAULT_COMMAND DEFINE_SYSTEM_ELEMENT FE VA !
DEFAULT_COMMAND REJECT_SYSTEM_CONSTITUENT LIQUID 2 C !
DEFAULT_COMMAND REJECT_PHASE LIQUID !
DEFAULT_COMMAND RESTOR_PHASE GAS !
```

DATABASE_INFORMATION

```
DATABASE_INFORMATION [text]*10000 !
```

This keyword defines a text for the detailed description of the current database. The text can be listed with the DATA command DATABASE_INFORMATION. An apostrophe (') can be used in the text to indicate a new line; and two apostrophes, (' ') can be used in the text to indicate a new line plus an empty line.



The continuous *text* length (each line with max 78 characters) is 10,000 characters.

EXAMPLE

```
DATABASE_INFORMATION This is the XXX-Alloy Solution Database '
    in the A-B-C-D-..... System. '
    Developed by TCS, released in May 2001. ''
... more ... !
```

TYPE_DEFINITION

```
TYPE_DEFINITION [data-type code]*1 [secondary keyword with
parameters] !
```

This keyword couples phases to an action performed by the DATA module when the DATA command ["GET_DATA" on page 126](#) is executed.

SECONDARY KEYWORDS

The secondary keywords and associated parameters in syntax are:

```
SEQ [filename]
RND# [filename]
GES [valid GIBBS command with parameters]
POLY3 [valid POLY command with parameters]
TDB [valid DATA command with parameters]
IF [conditional statement] THEN [keyword with parameters]
AFTER [valid GIBBS command with parameters]
```

The secondary keyword `SEQ` specifies a sequential file that stores parameters belonging to the phases using the associated data type code (which is defined by this keyword). A special case where the filename is given as an asterisk (*) implies that the database definition file also acts as a sequential data storage file. This case makes it possible to have a single file for a small database, which is especially suited for personal databases.

The secondary keyword `RND` should be concatenated with a positive integer # to indicate the type of the random file. Currently, there are these types of random files:

- `RND0`, the default, is used for complete Gibbs energy expressions (G0 parameters), where the search field is the unabbreviated parameter name.
- `RND1` is designated for functions, where the function name is used as the search field.

-
- `RND2` is reserved for binary interaction parameters, where its search field is also the unabbreviated parameter name without any interaction order notation.



Ternary and higher order interaction parameters must be specified on a sequential file. Moreover, the internal structures of these random files are subject to changes with different versions of DATA, and with implementations of DATA on various computer systems. For more information, see the FORTRAN program TDBSORT, which is available from Thermo-Calc Software AB.

The secondary keywords `GES`, `POLY3`, or `TDB` specifies a modification of, or addition to, phases having the associated data type code, such as magnetic contribution, another excess model, or any other valid GIBBS/POLY/DATA command that applies to a certain phase. By implementing this as a call to the interactive GIBBS/POLY/DATA module, flexibility is achieved. If a new type of addition is implemented in a GIBBS/POLY/DATA module, it can be immediately used in the database definition file without reprogramming the DATA module.



In several examples below, the use of the at (@) sign indicates any phase to which the relevant type definition (e.g. `A`, `B`, `4`, or `E`) applies.

The secondary keywords `IF` and `THEN` allow specification of a conditional statement structured with respect to the phase constitution that controls the execution of a following type-definition (keyword with parameters) string. See the last four examples.

The secondary keyword `AFTER` is similar to the `GES` keyword except the defined GIBBS command is executed after all parameters are entered. The reason for this is that the command has no effect unless there is a parameter. Following the `AFTER` keyword, a GIBBS command must be given and it is executed after entering the parameters of the phase.

The data-type code (always as one string) can be any normal or special character, e.g. `0`, `5`, `A`, `F`, `M`, `%`, `&`, and so forth, and is referred in the definition keywords ["PHASE" on page 9](#), ["COMPOUND_PHASE" on page 16](#) and ["ALLOTROPIC_PHASE" on page 16](#) for various phases.

A phase can have several `ADDITIONAL` parts of different types (that are enforced by certain `TYPE_DEFINITIONS` which call the GIBBS command `AMEND_PHASE_DESCRIPTION` for describing various contributions to Gibbs energy). However, the DATA/GIBBS module automatically deletes any early-defined `ADDITIONAL` part(s) of the same type.

The DATA module can selectively retrieve functions that are necessary for a defined system from a database that has functions stored in its `setup` file or `SEQ` sequential function file, while all other functions irrelevant for the defined system are ignored and are not saved in associated GIBBS and POLY workspaces.

EXAMPLES

```
TYPE_DEF % SEQ TCPATH\DATA\[DATABASE]\PARAMETERS.TDB !
TYPE_DEF I SEQ TCPATH\DATA\[DATABASE]\INTERACTION-PARAMS.TDB !
TYPE_DEF G RND0 TCPATH\DATA\[DATABASE]\GZERO-PARAMS.TDB !
TYPE_DEF F RND1 TCPATH\DATA\[DATABASE]\FUNCTIONS.TDB !
TYPE_DEF & RND2 TCPATH\DATA\[DATABASE]\BINARY-INTERACTIONS.TDB !
TYPE_DEF A GES AM_PH_DES @ MAGNETIC -1 0.40 !
TYPE_DEF B GES AM_PH_DES @ MAGNETIC -3 0.28 !
TYPE_DEF 4 GES AM_PH_DES @ EXCESS_MODEL REDLICH-KISTER_KOHLER !
TYPE_DEF 5 GES AM_PH_DES AQUEOUS EXCESS_MODEL HKF !
TYPE_DEF 6 GES AM_PH_DES AQUEOUS HKF_ELECTROSTATIC !
TYPE_DEF 7 GES AM_PH_DES AQUEOUS STATUS 02084000,,, !
TYPE_DEF 8 GES AM_PH_DES AQUEOUS MAJOR_CONST 1 H2O !
TYPE_DEF E AFTER AM_PH_DES LIQUID EXCESS MIXED-EXCESS
                A B LEGENDRE    C A POLYNOM ,,,, !
TYPE_DEF T AFTER AM_PH_DES LIQUID TERN-EXT TOOP-KOHLER  B A C ,,,,
!
TYPE_DEF Q AFTER AM_PH_DES LIQUID TERN-EXT KOHLER FE CR NI !
TYPE_DEF C IF (PD AND PT AND SN) THEN TDB RESTORE_PHASE BCT_A5 !
TYPE_DEF D IF (PD AND (PT OR SN)) THEN TDB REJECT_PHASE BCC_A2 !
TYPE_DEF E IF ((NB OR TI OR V) AND (C OR N)) THEN
    GES AM_PH_DES @ COMP_SET ,, CR NB TI V: C N: !
TYPE_DEF F IF (ALO3/2 OR CRO3/2 OR FEO OR MNO OR SIO2) THEN
    GES AM_PH_DES LIQUID COMP_SET ,, ALN%,ALO3/2%,CRO3/2%,
        FEO%,FEO3/2%,MNO3/2%,MNS%,SIO2%,TIO2% : !
TYPE_DEF R GES AM_PH_DES FE_LIQUID FRACTION_LIMITS Fe 0 0.6
    Ag 0 0.01 Al 0 0.05 Ca 0 0.05 Co 0 0.01 Cr 0 0.01
    Cu 0 0.02 Mg 0 0.05 Mn 0 0.05 Mo 0 0.05 Nb 0 0.05
    Ni 0 0.05 Pb 0 0.05 Si 0 0.10 Sn 0 0.02 Ti 0 0.05
    U 0 0.01 V 0 0.02 W 0 0.02 Zr 0 0.03
    B 0 0.01 C 0 0.01 H 0 0.01 N 0 0.01 O 0 0.01
    P 0 0.01 S 0 0.01 !
```

ORDERED PHASE RESTORES DISORDER CONTRIBUTION

When an ordered phase with disordered contribution is restored, the disordered contribution is automatically restored as well. You can also restore the disordered phase *without* restoring the ordered phase.



However the DIS_PART TYPE_DEFINITION must always be set on the ordered phase. It is important that the disordered phase is declared *before* the ordered phase. Otherwise it causes an error when DIS_PART TYPE_DEFINITION is executed and then either the ordered or disordered phase is rejected.

EXAMPLE

```
TYPE_DEFINITION & GES A_P_D FCC_A1 MAGNETIC -3.0 2.80000E-01 !
PHASE FCC_A1 %& 2 1 1 !

CONSTITUENT FCC_A1 :CR,NI% : C%,VA : !

$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM FCC_A1

TYPE_DEFINITION ' GES AMEND_PHASE_DESCRIPTION FCC_L12 DIS_PART
FCC_A1,,, !

TYPE_DEFINITION ( GES A_P_D FCC_L12 MAGNETIC -3.0 2.80000E-01
!

PHASE FCC_L12 %'( 3 .75 .25 1 !

CONSTITUENT FCC_L12 :CR,NI% : CR,NI% : C,VA% : !
```

For example a GES command such as the following only affects phases defined above or at the phase with this TYPE_DEFINITION in the TDB file:

```
TYPE_DEFINITION ( GES A_P_D FCC_L12 DIS_PART FCC_A1,,, !
```

For example a TDB command such as the following only affects phases defined *below* the phase with this TYPE_DEFINITION in the TDB file:

```
TYPE_DEFINITION ( TDB RESTORE_PHASE FCC_A1 !
```

FTP_FILE

```
FTP_FILE [filename] !
```

FTP_FILE is a special function random file and the function names correspond to the record numbers where these record names and the functions are stored. The FTP_FILE decreases search time for the associated database in the DATA module. The file is used for large substance databases along with a SEQ sequential or RND0 random file for storage of G0 parameters referring the functions named FxxxxT that are stored in the FTP file. The integer number xxxx is a search code used by DATA when such files are processed.



No modification of this file type is allowed.

EXAMPLE

```
FTP_FILE TCPATH\DATA\[DATABASE]\FTP-FILE.DATA !
```

FUNCTION

```
FUNCTION [function name]*8 [lowest temp. limit]
[expression 2]; [upper temp. limit 2] Y
[expression 1]; [upper temp. limit 1] Y
[expression 3]; [upper temp. limit 2] Y
..... ; ..... Y
[expression n-1]; [upper temp. limit n-1] Y
[expression n]; [upper temp. limit n] N {Ref. Index} !
```

GIBBS can use predefined functions in the expression (TP-Function) of a Gibbs energy parameter or in other functions. This is often used when several parameters (or functions) have a common sub-expression, such as for metastable modifications of elements. This keyword can appear in both files for database definition and sequential storage, but not in FTP files. A valid *function name* can have up to 8 characters.

A function always starts with a lowest temperature limit of its applicability, followed by one or more (up to 10) expressions (TP-Functions) that are coded as mathematical relations of constants, functions of stable variables (T and P) and other entered functions (normally with a # suffix, e.g. +3*GHSERAL#).

▶ ["ENTER_PARAMETER" on page 268](#)

The expression is a FORTRAN-like expression and operators +, -, *, = and ** can be used (** only with integer powers). Unary-functions LN or LOG (both for natural logarithm) and EXP (for exponential) can also be used. Each expression (TP-Function) should end with a semicolon (;), and be followed by its upper applicable temperature limit and a continuation indicator (Y to continue with the next expression or N to end the function's expression). If there is no continuation after a specific expression (TP-Function), the reference index can optionally be given after the N indicator.

A complete/valid function entry can be written in several continuation lines if the function's expression (TP-Function) is too long or if there is more than one applicable expression (TP-Function), as the maximum length of each line is 78 characters.



It is recommended to always have at least one empty space at the beginning of each continuation line. Otherwise, the DATA module may misunderstand the expression or issue some error messages when reading the function entry. Avoid entering functions like the one below.

```
FUNCTION GHSERXY 298.15  
-1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N !
```

Such a function is read by the DATA module as

```
1000+1058*T-38.9*T*LOG(T)+GFUNXY#
```

rather than

```
-1000+1058*T-38.9*T*LOG(T)+GFUNXY#
```

This is because the DATA module concatenates all lines and removes extra spaces before trying to enter the function in the GIBBS workspace. Thus, the – sign is taken as a delimiter between 298.15 and 1000, and the function incorrectly becomes:

```
FUNCTION GHSERXY 298.15 1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N  
!
```



Avoid this mistake by giving at least one empty space as the first character of a new line, such as

```
FUNCTION GHSERXY 298.15  
-1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N !
```

which is read correctly as

```
FUNCTION GHSERXY 298.15 -1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000  
N !
```

The lowest-temperature limit (in Kelvin) for the applicability of the (first) TP-Function in a function is normally set by default as 298.15 K, in most cases. However, you can set another limit when it is applicable (according to experimental data and assessments).

An upper-temperature limit (in Kelvin; followed by a Y or N sign) for the applicability of each TP-Function in a function must be given after the semicolon (;) immediately following the specific TP-Function. The highest-temperature limit (in Kelvin) for the applicability of the current function is always followed by the N sign. If a negative number is given as the lowest-temperature limit, it assumes there are breakpoints in pressure for this function. In these cases, it is interpreted as the lowest-pressure limit (in Pascal), and the other limits in the current function is also taken as pressure limit values (in Pascal).

The temperature/pressure limits for the functions are checked during calculations. An indicator is set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit. In these cases, an extrapolation is done using the TP-Function valid in the nearest temperature/pressure range.

The optional reference index *{Ref. Index}* is an integer number indicating where to find the particular function in a special reference file. The references are listed when doing the GET_DATA command in the DATA module. They can also be listed in the GIBBS module with the command LIST_DATA with the option R.



For accounting for the reference indices, also see the keyword ["REFERENCE FILE" on page 38](#).

The reference index field can also be an abbreviation (such as REF:250, REF_002, or REF-SGTE) which denotes the original reference. In this case, the reference cannot be obtained when issuing the DATA command GET_DATA or the GIBBS command LIST_DATA (with the option R).

However, the references directly coded in the database definition file (`***setup.TDB`) starting with a letter can be shown when issuing the DATA command GET_DATA or the GIBBS command LIST_DATA (with the option N or R). Normally, such references must be located after the LIST_OF_REFERENCE keyword. It is recommended to use reference code names such as REF001, REF018, etc. The reference list, which is generated by the GIBBS command ["LIST_DATA" on page 235](#) <file> with the N or R option, is also possible to be directly read by the DATA module.

The DATA module can selectively retrieve functions which are necessary for a defined system from a database that has functions stored in its setup file or SEQ sequential function file, while all other functions irrelevant for the defined system are ignored and are not saved in associated GIBBS and POLY workspaces. Previously, this can only be done for large databases that have functions stored in RND1 random or FTP function files.

EXAMPLES

```
FUNCTION GFREE 298.15 1000+GFUNXY#; 6000 N !
FUNCTION GFUNXY 298.15 -1000+200*T+30*T*LOG(T); 6000 N 505 !
FUNCTION G0_CAO 298.15 -663538.11+352.67749*T-57.7533*T*LN(T)
+5.3895E-03*T**2-8.879385E-07*T**3+575530*T**(-1);
1400.00 Y -625196.99+78.896993*T-20.40145*T*LN(T)
-1.112923E-02*T**2+5.1896733E-07*T**3-6917350*T**(-1);
2900.00 Y -499226.55-490.37695*T+51.95912*T*LN(T)
```

```

-2.961051E-02*T**2+1.4033905E-06*T**3-48114685*T**(-1);
3172.00 Y -587711.89+375.04117-62.76*T*LN(T);
6000.00 N REF020 !

```

PARAMETER

```

PARAMETER [GIBBS parameter name] [lowest temp. limit]
[expression 1]; [upper temp. limit 1] Y
[expression 2]; [upper temp. limit 2] Y
[expression 3]; [upper temp. limit 2] Y
..... ; ..... Y
[expression n-1]; [upper temp. limit n-1] Y
[expression n]; [upper temp. limit n] N {Ref. Index} !

```

This keyword can appear in both files for database definition and sequential storage, but not in FTP files. After the keyword, a valid *GIBBS parameter name* should be given.

It is used to define standard Gibbs energies (i.e. the **G** parameters for Gibbs energy of formations) of all valid end-members of various stoichiometric and solution phases, and excess Gibbs energies (i.e. the **L** parameters for Gibbs energy of interactions) of all binary, ternary, quaternary or higher-order interactions in various solution phases; both standard Gibbs energies and excess energies can also have parameters for contributions from PT-depended volume variations (i.e. the **V0**, **VA**, **VC** and **VK** parameters for molar volume, thermal expansivity, bulk modulus, isothermal compressibility and high-pressure fitting parameter), magnetic ordering (i.e. the **TC** and **BM** parameters for Curie temperature and Bohr magneton number) and hypothetical electrostatic interactions (i.e. **BM** parameter for Born functions $\omega_{Pr,Tr}$ of aqueous solute species).

The general form of a parameter is:

```

<identifier>(<phase>, <constituent array>; <digit>) <xxx>
<expression> <yyy> <keyword Y or N> <zzz> !

```

GENERAL FORM

| Name | Description |
|-------------------|----------------------------------------------|
| identifier | The parameter type. |
| phase | The phase name (maximum 24 characters). |
| constituent array | The specific constituent array in the phase. |

| Name | Description |
|----------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| digit | The degree of composition-dependent interaction contribution (an integer number from 0 to 9), that is only for excess energy (L), Curie temperature (TC) and Bohr magneton number (BMAGN), as well as for volume-related parameters (V0 or VA or VB or VC or VK); if it is valued as zero, or if it is for the standard Gibbs energy (G) for which the degree is always zero, it can be omitted. |
| expression | The mathematical relation to describe the parameter. |
| xxx and yyy | The low and high temperature limits respectively for the applicable temperature range of the parameter expression |
| keyword Y or N | The indicator on if there is continuation for the parameter expression or not |
| zzz | The reference index/number for the assessment of this parameter; |
| ! | The exclamation mark is used to indicate that the current parameter definition is ended |

GIBBS Parameter Name

The GIBBS parameter name has a general form of:

`<identifier>(<phase>,<constituent array>;<digit>)`

NAME EXAMPLES

| Parameter | Definition |
|--------------------|-------------------------------------------------------------|
| G (GAS, C1O2) | The Gibbs energy of formation of a CO2 molecule in gas. |
| G (FCC, Fe:VA) | The Gibbs energy of formation of fcc Fe with interstitials. |
| L (LIQ, Fe, Cr; 0) | The regular solution parameter for Fe and Cr in liquid. |
| L (LIQ, Fe, Cr; 1) | The sub-regular solution parameter. |
| TC (BCC, Fe:Va) | The Curie temperature of bcc Fe. |
| BMAGN (BCC, Fe:Va) | The Bohr magneton number parameter of bcc Fe. |

The GIBBS parameter name consists of several parts. The first is a *type-identifier*. The following type-identifiers are legal:

| Type-Identifier | Definition |
|-----------------|----------------------------------------------------------------------------------------------------------|
| G | Standard energy parameter (Gibbs energy of formation) |
| L | Excess energy parameter (Gibbs energy of interaction) |
| TC | Curie temperature for magnetic ordering |
| BMAGN or BM | Bohr magneton number for magnetic ordering (or Born function ω Pr,Tr for aqueous solute species). |
| V0 | Molar volume at 298.15 K and 1 bar (a numeric value only) |
| VA | Integrated thermal expansivity $\int_{298.15}^T \alpha(T) dT$ |
| VC | High-pressure fitting parameter |
| VK | Isothermal compressibility |

You can also use **G** for interaction parameters; and on output list (performed by the GIBBS command LIST_PARAMETER or LIST_PHASE_DATA) the type-identifier **L** is always used for interaction parameters. Note that the type-identifier **BM** is also used for Born functions ω Pr,Tr of aqueous solute species.

The identifier must be followed by an opening parenthesis, a phase name, a comma and a constituent array. Optionally, the constituent array can be followed by a semicolon and a digit. The parameter name is terminated by a closing parenthesis.



It is important that if a phase bears a legal phase-type (among **G**, **A**, **Y**, **L**, **I**, **F** and **B**) in its phase definition (already by the PHASE keyword; such as **GAS:G**, **LIQUID:L**, **SLAG:L**, **IONIC_LIQ:Y**, **SPINEL:I**, **FCC_L12:F**, **HCP_D021:F**, **BCC_B2:B**, **AQUEOUS:A**), such a valid phase-type code should not be attached to the phase name in the PARAMETER keyword.



Specifying the phase name in UPPER-case is recommended. You can define a phase name as a mixture of UPPER-case and lower-case letters in a database, but the DATA module automatically converts all lower-case to UPPER-case because the GIBBS module only recognizes UPPER-case phase names.

The *constituent array* consists of a list of constituent names. Interaction parameters have two or more constituents from the same sublattice separated by a comma. If the phase has sublattices, at least one constituent in each sublattice must be specified. The exception is if the phase is ionic liquid (specified with the "phase bit" **:Y**), then neutral endmember and

interaction parameters are written as if the first sublattice does not exist, e.g. `PARAM G (IONIC_LIQ, FeO3/2;0)`, i.e. the constituent array does not contain any constituents from the first (cation) sublattice.

► For more ionic liquid specific parameters, see ["Parameters for the Two Sublattice Ionic Liquid Model" on page 32](#).

The constituents in different sublattices must be given in sublattice order and are separated by a colon.

After the component array, a sub-index digit can be specified after a semicolon. This digit must be in the range 0 to 9. The interpretation of the sub-index depends on the excess energy model used for the phase. If no semicolon and digit are given, the sub-index value is assumed to be as zero.

The excess energy parameters, e.g. the regular/subregular (binary) parameter or ternary parameters, are multiplied with two or more fractions of the constituents from the same sublattice of the solution phase. These additional constituents must be given as interacting constituents.



Be careful about the sign of odd terms, for example, `L(BCC, B, A:VA;1)` is treated as `L(BCC, A, B:VA;1)`, i.e. it is always put into alphabetical order.



Solution phases with sublattices may have interacting constituents in each sublattice.

You can use an asterisk (*) to denote that the excess interaction parameter is independent of the constituents of a specific sublattice. For example, `L(FCC_L12, AL, NI:*)` means that the interaction parameter is for the binary interaction between constituents AL and NI on the first sublattice in the FCC_L12 solution phase, while it is independent of all constituents on the second sublattice. A interaction parameter in the list of constituents is always added to the Gibbs energy and the asterisk (*) is calculated with the term of $[1 - \sum y(\text{specified constituents})]$, which implies that in an A-B binary system the following three `L` parameters are identical (but in higher-order systems, they are different):

- `L(phase, A, B)` is multiplied with $x(A) * x(B)$
- `L(phase, A, *)` is multiplied with $x(A) * (1 - x(A))$
- `L(phase, B, *)` is multiplied with $x(B) * (1 - x(B))$

A parameter always starts with a lowest temperature limit of its applicability, followed by one or more (up to 10) expressions (TP-Functions) coded as mathematical relations of constants, functions of stable variables (T and P) and entered functions (normally with a # suffix, e.g. +3*GSERAL#).

The expression is a FORTRAN-like expression and operators +, -, *, = and ** can be used (** only with integer powers). Unary-functions LN or LOG (both for natural logarithm) and EXP (for exponential) can also be used. Each expression (TP-Function) should end with a semicolon (;) and be followed by its upper applicable temperature limit and a continuation indicator (Y to continue with the next expression, or N to end the parameter's expression). If there is no continuation after a specific expression (TP-Function), the reference index can be optionally given after the N indicator.

A complete/valid parameter entry can be written in several continuation lines if the parameter's expression (TP-Function) is too long or if there is more than one applicable expression (TP-Function), as the maximum length of each line is 78 characters.



It is recommended to always have at least one empty space at the beginning of each continuation line. Avoid entering parameters such as:

```
PARAMETR G(LIQUID,A,B) 298.15  
-2000+4568*T+2*GFUNAB#; 6000 N !
```

Such a parameter is read by the DATA module as 2000+4568*T+2*GFUNAB#, rather than as -2000 +4568*T+2*GFUNAB#.



Avoid this mistake by giving at least one empty space as the first character of a new line, such as

```
PARAMETR G(LIQUID,A,B) 298.15  
-2000+4568*T+2*GFUNAB#; 6000 N !
```

The lowest-temperature limit (in Kelvin) for the applicability of the (first) TP-Function in a parameter is normally set by default as 298.15 K, in most cases; however, you can set another limit when it is applicable (according to experimental data and assessments). An upper-temperature limit (in Kelvin; followed by a Y or N sign) for the applicability of each TP-Function in a parameter must be given after the semicolon (;) immediately following the specific TP-Function; and the highest-temperature limit (in Kelvin) for the applicability of the current parameter is always followed by the N sign. If a negative number is given as the lowest-temperature limit, it is assumed that there are breakpoints in pressure for this parameter. In such cases, it is interpreted as the lowest-pressure limit (in Pascal), and the other limits in the current parameter are also taken as pressure limit values (in Pascal).

The temperature/pressure limits for the parameters are checked during calculations. An indicator is set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit. In these cases, an extrapolation is done using the TP-Function valid in the nearest temperature/pressure range.

The optional reference index *{Ref. Index}* is an integer number indicating where to find the particular parameter in a special reference file. The references are listed when doing the GET_DATA command in the DATA module. These can also be listed in the GIBBS module with the command LIST_DATA and the option R or N.



For accounting the reference indices, also see the keyword ["REFERENCE_FILE"](#) on page 38.

The reference index field can also be an abbreviation (such as REF:250, REF_002, or REF-SGTE) denoting the original reference. In this case, the reference cannot be obtained when issuing the DATA command GET_DATA or the GIBBS command LIST_DATA (with the option R or N).

However, the references directly coded in the database definition file (`***setup.TDB`) that starts with a letter can be shown when issuing the DATA command GET_DATA or the GIBBS command LIST_DATA (with the option R or N). Normally, such references must be located after the LIST_OF_REFERENCE keyword. It is recommended to use reference code names such as REF001, REF018, etc. The reference list, which is generated by the GIBBS command LIST_DATA <file> with the N option, is thus also possible to be directly read by the DATA module.

EXAMPLES

```
PARAMETER G(BCC,FE:VA) 298.15 1000+200*T+...; 6000 N 91DIN !
PARAMETER TC(BCC,FE:VA) 298.15 +1043; 6000 N 91DIN !
PARAMETER BMAGN(BCC,FE:VA) 298.15 +2.22; 6000 N 91DIN !
PARAMETER G(SIGMA,FE:CR:CR;0) 298.15 1000+200*T+...; 6000 N 101 !
PARAMETER G(LIQUID,AL;0) 298.15 +11005.553-11.840873*T
+7.9401E-20*T**7+GHSERAL#;
933.60 Y +10481.974-11.252014*T+1.234264E+28*T**(-9)+GHSERAL#;
2900.00 N REF:283 !
PARAMETER G(BCC_A2,PB:C) 298.15 UN_ASS#; 300 N REF:0 !
PARAMETER G(BCC_A2,NI:C;0) 298.15 +GHSERNI#+3*GHSERCC#
+400000-100*T; 6000 N REF071 !
```

```

PARAMETER G(BCC_A2,MN:VA) 298.15 +GMNBCC#; 6000 N REF285 !
PARAMETER BM(AQUEOUS,OH-1) 298.15 +Z0002PW0#; 1600 N 155 !
PARAMETER L(BCC,FE,CO:VA;0) 298.15 1000+200*T+...; 6000 N !
PARAMETER L(BCC,FE,CO:VA;1) 298.15 1000+200*T+...; 6000 N !
PARAMETER L(BCC,FE,CO:VA;2) 298.15 1000+200*T+...; 6000 N !
PARAM TC(BCC_A2,CO,MO:VA;0) 298.15 -3700; 6000 N R454 !
PARAM TC(BCC_A2,CO,MO:VA;1) 298.15 +2300; 6000 N R454 !
PARAM BMAGN(BCC_A2,CO,MO:VA;0) 298.15 -3.445; 6000 N R454 !
PARAM V0(BCC_A2,CR,FE:VA;0) 298.15 +ZERO#; 6000 N REF06V !
PARAM V0(BCC_A2,CR,FE:VA;1) 298.15 -1.10524097E-7; 6000 N REF06V !
PARAM V0(BCC_A2,CR,FE:VA;2) 298.15 +1.40024130E-7; 6000 N REF06V !
PARAM VA(BCC_A2,CR,FE:VA;0) 298.15 -6.49444634E-6*DELTAT#; 6000 N
REF06V !
PARAM VA(BCC_A2,CR,FE:VA;1) 298.15 +2.91269321E-5*DELTAT#; 6000 N
REF06V !

```

Parameters for the Two Sublattice Ionic Liquid Model

For the two sublattice ionic liquid model (specified with the "phase bit" :Y in the phase declaration), there are some additional requirements on the allowed parameters. While in the regular case all combinations of a phase's constituents are allowed as end-members, there are some constraints on the allowed parameters for ionic liquid.

In the ionic liquid model, the vacancy has been given an "induced" charge $-Q$, where Q is the average charge of the first (cation) sublattice.

All allowed parameters are listed below. The following notations are used:

- C = Cation
- C1 = Cation 1 if more than one. Similar for anions and neutrals.
- A = Anion
- VA = Vacancy
- N = Neutral
- D = Anion or vacancy or neutral (i.e. anything on the second sublattice)

The phase description is:

$$(C1, C2 \dots Ci) P(A1, A2 \dots Ai, VA, N1, N2 \dots Ni) Q$$

In the ionic liquid model, the *vacancy* has been given an "induced" charge $-Q$, where Q is the average charge of the first (cation) sublattice.

Allowed end-members, assuming the phase name is IONIC_LIQ:

```
G ( IONIC_LIQ, C:A; 0 )
G ( IONIC_LIQ, C:VA; 0 )
G ( IONIC_LIQ, N; 0 )
```

(The last line is an exception to the case that the constituent array must contain constituents from all sublattices)

This leaves one not allowed end-member:

```
G ( IONIC_LIQ, C:N; 0 )
```

Allowed binary interaction parameters, where i is the interaction order in a Redlich-Kister expansion.

```
G ( IONIC_LIQ, C1, C2:A; i )
G ( IONIC_LIQ, C1, C2:VA; i )
G ( IONIC_LIQ, C:VA, N; i )
G ( IONIC_LIQ, N1, N2; i )
G ( IONIC_LIQ, C:A1, A2; i )
G ( IONIC_LIQ, C:A, VA; i )
G ( IONIC_LIQ, C:A, N; i )
```

No other binary interactions are allowed.

Allowed ternary interaction parameters. The interaction is composition independent if there is one parameter with $i = 0$. It is composition dependent if there are three parameters with $i = 0, 1$ and 2 . There can only be one or three parameters for one combination of constituents

```
G ( IONIC_LIQ, C1, C2, C3:A; i )
G ( IONIC_LIQ, C1, C2, C3:VA; i )
G ( IONIC_LIQ, N1, N2, N3; i )
G ( IONIC_LIQ, C1, C2:VA, N; i )
G ( IONIC_LIQ, C:VA, N1, N2; i )
G ( IONIC_LIQ, C:A, D1, D2; i )
G ( IONIC_LIQ, C1, C2:A, D; i )
```

No other ternary interactions are allowed.

OPTIONS

```
OPTIONS /[alloy name]([composition limitations for all alloying
elements]) !
```

This keyword defines an alloy in a database. An alloy has a name, a major component and a number of alloying elements. The purpose for defining an alloy is to be able to tell you about applicable composition limits of the current database in applications to that particular type of alloy. It is possible to have several alloys in the same database. The alloys are given after the keyword in the database.

The alloy name must be preceded by a slash (/) and terminated by the opening parenthesis, with no spaces are allowed in between.

- The alloy name is maximum 8 characters.
- After the parenthesis, follows the major element and a parenthesis with its minimum mass and minimum mole percent given inside.
- Then, the alloying element names, each with its maximum mass and mole percent are given within parenthesis.
- There must a space between definitions for each alloying element.
- The alloy definition is terminated by a closing parenthesis, and the whole OPTIONS keyword by the exclamation mark (!).

EXAMPLE

```
OPTIONS /SSteel(Fe(60,60) CR(30,30) NI(15,15) SI(1,1) N(.1,1)) !
```

TABLE



It is recommended to always have at least one empty space at the beginning of each continuation line. Otherwise, the DATA module may issue some error messages when reading the table entry.

```
TABLE [name]*8 [start temp] [end temp] [delta temp] [table values]  
!
```

This keyword can appear in both files for database definition and sequential storage, but not in FTP files. It makes a table of Gibbs energy as a function of temperature where the values are given from the start temperature to the end temperature, at a step of the delta temperature.

EXAMPLE

```
TABLE DMTAB 1000.0 1500.0 100.0 -2912.9008 -2834.2416 -2755.5824  
-2677.7600 -2600.7744 -2524.2072 !
```

ASSESSED_SYSTEMS

```
ASSESSED_SYSTEM [descriptions on special treatments for specific  
assessed systems]*8000 !
```

This keyword can be included in the database definition file (the `***setup.TDB` file). A maximum of 8000 characters after the keyword (to describe some special options when the DATA, GIBBS and POLY models deal with the existing systems with assessed data) is allowed until the exclamation mark (!).

Several ASSESSED_SYSTEMS keywords can be used in the same TDB file in order to have more lists of assessed systems. There is no limit to the number of the entries in the same TDB file.

The assessed systems in the database, and the special treatment options, are typed after the keyword. The elements (always in UPPER CASE) in each assessed system must be in alphabetical order and be separated by a hyphen, such as C-FE for the Fe-C binary system, and C-CR-FE for the Fe-Cr-C ternary system. A space must be between each assessed system. Information on assessed binary, ternary or higher-order systems may also be given in this way.



A ternary system like C-CR-FE does not imply that the binary C-CR, C-FE and CR-FE are assessed. There is no way to indicate partially assessed systems.

- There is a field to give some descriptive information for a specific system, with various options about how to:
- Reject or restore phase(s) from the current database in the DATA module;
- Set major constituent(s) in the first composition set and to set a second composition set for a specific phase available in the current database in the GIBBS module; *and*
- Calculate this specific system in the POLY module.
- This is the facility used by the BIN (binary phase diagrams) and TERN (ternary phase diagrams) modules in the Thermo-Calc software/database package.

The descriptive information must immediately follow the specific system name, and must be enclosed within parenthesis (and), and the left parenthesis must follow directly after the system, such as :

```
AL-NI (TDB +L12 ;G5 C-S:L12/NI:AL:VA ;P3 STP:.8/1200/1
STP:.2/600/1)
```

The syntax TDB means that the commands to the DATA module proceed, and +L12 in the example means that the phase called L12 should be restored (it has been rejected by default).

The directive ;G5 means that the following are commands to the GIBBS module. C_S: means creating a second composition set, after the colon follows the phase name and after the slash the major constituents.

After the directive ;P3 follows commands to the POLY module. STP: means setting a start point with the value of the X-axis first (composition for the second element in a binary system), the slash separates the Y-axis value (temperature), and possibly one or more directions (-1, 1, -2 or 2).

A summary of the allowed syntax is:

TDB accepts

- +phase and -phase for restore/reject.
- ;G5 accepts
 - MAJ:phase/constituent-array for major constituents of the first composition set.
 - C_S:phase/constituent-array for a second composition set.
- ;P3 accepts
 - TMM:lt/ht for the low-/high-temperature limits (lt and ht; for instance TMM:500/4000) suitable for calculating phase diagrams and property diagrams of a binary system.
 - * for a default start point which is set as:
 - for a binary system: at the composition $X(2^{\text{nd}} \text{ element}) = .1234$, temperature $T = 1100 \text{ K}$ and with the default directions; or
 - for a ternary system: at the compositions $X(2^{\text{nd}} \text{ element}) = .1234$ and $X(3^{\text{rd}} \text{ element}) = .1234$ and with the default directions.
 - STP:x/t/d1/d2/d3 for a specific start point in a binary system which is set as at the composition $X(2^{\text{nd}} \text{ element}) = x$ and temperature $T = t$ (in K), and with the directions d1, d2 and/or d3.
 - STP:x1/x2/d1/d2/d3 for a specific start point in a ternary system which is set as at the compositions $X(2^{\text{nd}} \text{ element}) = x1$ and $X(3^{\text{rd}} \text{ element}) = x2$ and with the directions d1, d2 and/or d3.

- The direction(s) can be defined as -1, 1, -2 or 2. If no direction is specified, all default directions are used (meaning no ADD command is enforced in the POLY module).
- If only one start point is specified, the direction(s) may be omitted; if more than one start points are specified, at least one direction for each start point must be given for all start points.

Each entry for a specific binary or ternary sub-system can be written in one or several lines (each line with 78 characters).

OTHER EXAMPLES

```

ASSESSED_SYSTEMS
AL-NI (TDB +L12 +BCC_B2 ;G5 C_S:L12/NI:AL:VA
      ;P3 STP:.8/1000/1 STP:.45/700/1 STP:.7/700/1)
AL-PB (TDB -HCP -BCC
      ;G5 MAJ:LIQ/AL MAJ:FCC/AL:VA C-S:LIQ/PB C-S:FCC/PB:VA ;P3
*)
CR-FE (;G5 C-S:BCC/CR:VA ;P3 STP:.6/1200/1/-2/2)
AG-CU (;G5 MAJ:FCC/AG:VA C_S:FCC/CU:VA ;P3 STP:.3/1000)
C-NB (;P3 STP:.9/1100/1)
C-SI (;P3 *)
CO-CR (;G5 MAJ:FCC/CO:VA C_S:FCC/CR:VA ;P3 STP:.1/1100)
CR-FE (TDB -HCP ;G5 C_S:BCC/CR:VA ;P3 STP:.6/1200/1/-2/2)
CR-NI (;P3 *)
CR-W (;G5 MAJ:BCC/W:VA C_S:BCC/CR:VA
      ;P3 TMM:500/4000 STP:.3/700/1 STP:.3/1800/2 )
CU-FE (TDB -HCP ;G5 MAJ:LIQ/CU MAJ:FCC/FE:VA C_S:FCC/CU:VA
      ;P3 STP:.9/1400)
FE-N (TDB +FE4N ;P3 *)
FE-O (TDB -LIQUID +IONIC ;G5 C_S:ION_LIQ/FE+2:O-2 MAJ:ION_
LIQ/FE+2:VA
      ;P3 STP:.2/2000/1 )
FE-S (TDB -LIQUID +IONIC ;G5 C_S:ION_LIQ/FE+2:S MAJ:ION_LIQ/FE+2:S-
2 ;P3 *)
AL-MG-SI (;P3 *)
C-CR-FE ;G5 MAJ:BCC/FE:VA C_S:BCC/CR:VA ;P3 *) !

```



The semicolon (;) is a part of the ;G5 and ;P3 directives. A long descriptive information can be written in more than one line, such as for the AL-NI, AL-PB, CU-FE and FE-O systems shown above.

The directive ;P3 * is needed if the default start point should be used. If there is no P3 directive, the BIN or TERN module generates some 20 different start points in order to cover all possible compositions and temperatures (for a binary system) or all possible compositions (for a ternary system under any specific temperature).

REFERENCE_FILE

```
REFERENCE_FILE [file name] !
```

This keyword takes a reference file name as its argument. This reference file (that must be edited in a restrictive way and be saved as a blocked file with a fixed line-length for each line in the file, as described below) contains a complete list of the references for the various parameters (and sometimes functions) in the database. The file must have a fixed record structure: each reference entry with one or several records, and each record with exactly 78 characters written in one single blocked line; and no empty space is allowed at the beginning of all lines in the file. If there are more than one record entered for a reference entry, all the continuation lines must start with an ampersand (&). The line number of the first record for a specific reference entry is then accounted as the unique integer for that specific reference, which is referred when a parameter or function calls this integer as the optional {Ref. Index}.



Also see keyword ["PARAMETER" on page 26](#) or ["FUNCTION" on page 23](#) about specifying a reference index.

EXAMPLE

```
/-1<G>                T.C.R.A.S. Class 1
AG1.64TE1            THERMODATA 01/93
&28/01/93
&SILVER 1.64-TELLURIDE. Solid Standard State.
AG1                  HULTGREN SELECTED VAL.          SGTE **
&AT.WEIGHT 107.870,STANDARD STATE:CODATA KEY VALUE.MPT=1234.93K.
&--U.D. 30/10/85.
AG1<G>                T.C.R.A.S. Class: 1
AG1/+1<G>            T.C.R.A.S. Class: 1
AG1BR1              N.P.L.                          SGTE **
```

```

&Tfusion uncertain and heat vaporization estimated.
AG1BR1<G>          THERMODATA 01/93
&28/01/93
&Gaseous Standard State.
AG1BR1O3          BARIN & KNACKE.SUPPL.REF:62,* SGTE **
&AGO3BR    SILVER OXYTRIBROMIDE

```

In the example, the unique integers of related references (for assessed elements, species, phases, interactions, etc.) are:

```

1/-1<G>
2AG1.64TE1
5 AG1
8AG1<G>
9AG1/+1<G>
10AG1BR1
12AG1BR1<G>
15AG1BR1O3

```

LIST_OF_REFERENCE

```

LIST_OF_REFERENCE
NUMBER SOURCE
    [REFxxx]  '[Detailed reference]'
.....
..... !

```

This keyword starts a reference list that is directly coded in the database definition file (`***setup.TDB`). Its argument begins on the following line, and normally has an explanation line (NUMBER SOURCE) that is followed by various reference codes. Each reference code may occupy one or more lines (each line with maximum 78 characters), but must have a reference code name (that starts with a letter) and the detailed reference information (that is written within two single-quotation marks, `' '`). It is recommended to use reference code names such as `REF001`, `REF018`, etc. A maximum of 400,000 characters after the keyword is allowed until the exclamation mark (`!`).

Such a reference list can be shown when issuing the DATA command ["GET_DATA" on page 126](#) or the GIBBS command ["LIST_DATA" on page 235](#) (with the `R` option). The reference list, which is generated by the GIBBS command `LIST_DATA <file>` with the `N` option, has this structure, and is thus possible to be directly read by the DATA module.

EXAMPLE

```
LIST_OF_REFERENCES
NUMBER  SOURCE
REF283  'Alan Dinsdale, SGTE Data for Pure Elements,
        Calphad Vol 15(1991) p 317-425,
        also in NPL Report DMA(A)195 Rev. August 1990'
REF224  'P-Y Chevalier, Thermochemica Acta, 130 (1988) p 33-41; AG-
SI'
!
```

ADD_REFERENCE

```
ADD_REFERENCE
[REFxxx] '[Detailed reference]'
.....
..... !
```

Use this keyword to have an unlimited number of references. The use of this is the same as that of ["LIST_OF_REFERENCE" on the previous page](#), and is used after it. Several `ADD_REFERENCE` sections can be used in a single database if there are too many references.

It is recommended to always start with a so-called *empty reference* (such as the `DUMP0` reference in the following example) as the first entry in each of the `ADD_REFERENCE` sections to make sure that all references are listed appropriately as retrieving data by issuing the ["GET_DATA" on page 126](#) command.

EXAMPLE

```
ADD_REFERENCE
DUMP0  'Empty reference 0'

REF4  'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-
92

      TRITA 0270 (1986); CR-FE'

REF5  'J-O Andersson, Met. Trans A, Vol 19A, (1988) p 627-636

      TRITA 0207 (1986); C-CR-FE'

REFS  'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys
Database,

      v1.2; Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters
```

```

        at high temperatures.'

    ... ..

!
ADD_REFERENCE
    DUMP1 'Empty reference 1'

    REF275 'A. Fernandez Guillermet, Z. Metallkde. Vol 79(1988)
p.524-536,
        TRITA-MAC 362 (1988); C-CO-NI AND C-CO-FE-NI'

    REF393 'K. Frisk, Metall. Trans. Vol 21A (1990) p 2477-2488,
        TRITA 0409 (1989); CR-FE-N'

    REF1096 'P. Gustafson, Metall. Trans. 19A(1988) p 2547-2554,
        TRITA-MAC 348, (1987); C-CR-FE-W'

    ... ..

!

```

CASE and ENDCASE

```

CASE [ELEMENT/SPECIE/PHASE] !
    IF (boolean algebra on element, species or phase names) THEN
        [GIBBS/POLY/DATA command] !
ENDCASE !

```

This keyword takes as its argument, a definition on which type of the following Boolean algebra operates. A simple Boolean algebra using **AND** and **OR** with a maximum of four levels of parentheses works. The **CASE** construction must end with the **ENDCASE** keyword. This makes it possible to have additional GIBBS or POLY commands executed depending on the user selection of elements, species or phases. The DATA commands that can be given as secondary keyword to ["DEFAULT_COMMAND" on page 17](#) can also be executed.

EXAMPLE 1

```

CASE ELEMENT !
    IF ((CR OR TI OR V) AND N)
        THEN GES AM_PH_DES @ C_S ,, CR MO TI V:C N: !
ENDCASE !

```

EXAMPLE 2

```

CASE ELEMENT !

```

```
        IF(O) THEN TDB DEFINE_SYSTEM_ELEMENT /- !  
    ENDCASE !
```

EXAMPLE 3

```
    CASE ELEMENT !  
        IF(AL AND FE)  
            THEN TDB DEF_SYS_ELEMENT VA !  
    ENDCASE !
```

VERSION_DATA

```
VERSION_DATE [string]*78 !
```

The string is denoted as the version/revision date and database manager of the database. Nowadays, this directive is used mainly for the purpose of keeping the development and revision history mostly updated.

EXAMPLE

```
VERSION_DATE Last update and adjustment: Database Manager, 2015-  
09-25 !
```

Working with the Mobility Databases

In this section:

| | |
|-----------------------------------------------------|----|
| Extensions to Database Definition File Syntax | 44 |
| PARAMETER | 44 |
| DIFFUSION | 45 |
| ZEROVOLUME_SPECIES | 46 |

Extensions to Database Definition File Syntax

Software packages for simulation of diffusional phase transformations, such as the Diffusion Module (DICTRA) and Precipitation Module (TC-PRISMA), need both thermodynamic data and kinetic data (i.e. diffusivities or mobilities). Naturally, the handling and storage of kinetic data also benefits from the use of some kind of database management. Thus, the TDB database definition file syntax has been extended to incorporate some new keywords needed for storing kinetic data - ["PARAMETER" on page 26](#), ["DIFFUSION" on the next page](#), and ["ZEROVOLUME_SPECIES" on page 46](#).

PARAMETER

```
PARAMETER [special GIBBS parameter name] [low temp. limit]
[expression 1]; [upper temp. limit 1] Y
[expression 2]; [upper temp. limit 2] Y
[expression 3]; [upper temp. limit 2] Y
..... ; ..... Y
[expression n-1]; [upper temp. limit n-1] Y
[expression n]; [upper temp. limit n] N {Ref. Index} !
```

This keyword allows you to enter all types of normal GIBBS parameters for thermodynamic data as well as five special extensions suitable for kinetic data used in the Diffusion Module (DICTRA).

Valid extensions to special GIBBS parameter names are:

- **MQ**: Activation enthalpy for mobility equation.
- **MF**: Pre-exponential factor for mobility equation.
- **DQ**: Activation enthalpy for diffusivity equation.
- **DF**: Pre-exponential factor for diffusivity equation.
- **VS**: Volume counted per mole of volume carrying species.

EXAMPLE



See the TDB file for example exa4.

```

$===== D I F F U S I O N   D A T A =====
$
ZEROVOLUME_SPECIES C VA !

PARA DQ(FCC_A1&C,*,*),, -148000+32.8*T+R*T*LOG(4.53E-7);,,N!
PARA DQ(FCC_A1&FE,*,*),, -286000+R*T*LOG(0.700E-4);,,N!

```

DIFFUSION

DIFFUSION [model keyword] [phase name] [additional parameter(s)] !

This keyword specifies the type of diffusion model to use for a phase if the default model is not desired. The default model calculates the full diffusion matrix. A diffusivity is calculated from the different mobilities and the thermodynamic factors. The former ones are calculated as:

$$M = \exp \left(\sum MF/RT \right) \exp \left(\sum MQ/RT \right) / RT$$

where \sum stands for a weighted summation of the different MF's and MQ's plus possibly a Redlich-Kister term.

VALID MODEL KEYWORDS

| Keyword | Description |
|----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| NONE | No diffusion in this phase |
| DILUTE | Constitution list of dependent species in each sublattice must be given as an additional parameter. Only the diagonal terms in the diffusion matrix are calculated. $D = \exp(\sum DF/RT) \exp(\sum DQ/RT)$. |
| SIMPLE | Constitution list of dependent species in each sublattice must be given as additional parameter. Only the diagonal terms in the diffusion matrix are calculated. $D = \sum DF + \sum DQ$. |
| MAGNETIC | The so-called ALPHA and ALPHA2 parameters must be given as additional parameters. ALPHA is for the substitutional magnetic model and ALPHA2 for the interstitial one. By appending an & sign and a species name after the alpha keyword one can supply individual values for the different species. The full diffusion matrix is calculated. |

EXAMPLES

```
DIFFUSION NONE SIGMA !  
DIFFUSION DILUTE CEMENTITE : FE : C : !  
DIFFUSION MAGNETIC BCC_A2 ALPHA=0.3 ALPHA2&C=1.8 ALPHA2&N=0.6 !
```

ZEROVOLUME_SPECIES

```
ZEROVOLUME_SPECIES [list of species] !
```

In the Diffusion Module (DICTRA), the assumption that the volume is carried by the substitutional elements only is applied. The interstitial elements are assumed to have zero molar volumes. This keyword uses a list of which species are to be considered as zero volume ones for an argument.



There is no underscore (_) between *Zero* and *Volume*.

EXAMPLE

```
ZEROVOLUME_SPECIES VA C N !
```

Database Definition File Examples

In this section:

| | |
|-------------------------------------------------------------------|----|
| Example 1: A Steel Database | 48 |
| Example 2: A Custom Database for the Sb-Sn Binary System | 49 |
| Example 3: A Public Database for the Fe-Cr-C Ternary System | 52 |

Example 1: A Steel Database

```
TEMP-LIM 500.0 2000.0 !

$

$ELEMENT, NAME, REF.STATE, ATOMIC-MASS, H0, S0 !

ELEMENT VA VACUUM          0.0    0.0 0.0 !
ELEMENT C  GRAPHITE        12.011  0.0 0.0 !
ELEMENT V   BCC             50.9415 0.0 0.0 !
ELEMENT CR  BCC-PARAMAGNETIC 51.996  0.0 0.0 !
ELEMENT FE  FCC-PARAMAGNETIC 55.847  0.0 0.0 !
ELEMENT NI  FCC-PARAMAGNETIC 58.69   0.0 0.0 !
ELEMENT MO  BCC             95.94   0.0 0.0 !
ELEMENT W   BCC             183.85   0.0 0.0 !

$

$PHASE, NAME, TYPE, NR-OF-SUBL, SITES-IN-EACH-SUBL. !

PHASE BCC      B1M  2 1.0 3.0 !
PHASE FCC      F2M  2 1.0 1.0 !
PHASE HCP      0    2 2.0 1.0 !
PHASE LIQUID   3    2 1.0 1.0 !
PHASE CEMENTITE 4    2 3.0 1.0 !
PHASE M23C6    4    2 23.0 6.0 !
PHASE M7C3     4    2 7.0 3.0 !
PHASE M6C      4    4 2.0 2.0 2.0 1.0 !
PHASE SIGMA    0    3 10.0 4.0 16.0 !
PHASE MU-PHASE 0    3 7.0 2.0 4.0 !
PHASE R-PHASE  0    3 27.0 14.0 12.0 !
PHASE GRAPHITE 4    1 1.0 !

$

$CONSTITUENT, PHASE-NAME : CONSTITUENTS !

CONSTITUENT BCC :V CR FE NI MO W:VA C: !
CONSTITUENT FCC :V CR FE NI MO W:VA C: !
CONSTITUENT HCP :CR FE NI:VA C N: !
CONSTITUENT LIQUID :C V CR FE NI MO W VA:VA C: !
CONSTITUENT CEMENTITE :CR FE:C: !
CONSTITUENT M23C6 :CR FE:C: !
CONSTITUENT M7C3 :CR FE:C: !
CONSTITUENT M6C :FE:W:FE W:C: !
```

```

CONSTITUENT SIGMA :FE:V CR MO:FE V CR MO: !
CONSTITUENT MU-PHASE :FE:MO W:FE MO W: !
CONSTITUENT R-PHASE :FE:MO :FE MO: !
CONSTITUENT GRAPHITE :C: !

$
$TYPE_DEFINITIONS:
TYPE-DEFINITION 0 SEQ TCPATH\DATA\METDATA\TC-THEREST.TDB !
TYPE-DEFINITION 1 SEQ TCPATH\DATA\METDATA\TC-BCC.TDB !
TYPE-DEFINITION 2 SEQ TCPATH\DATA\METDATA\TC-FCC.TDB !
TYPE-DEFINITION 3 SEQ TCPATH\DATA\METDATA\TC-LIQUID.TDB !
TYPE-DEFINITION 4 SEQ TCPATH\DATA\METDATA\TC-CARBIDES.TDB !
TYPE-DEFINITION M SEQ TCPATH\DATA\METDATA\TC-CURIE-BOHR.TDB !
TYPE-DEFINITION B GES AM-PH BCC MAGNETIC -1 .4 !
TYPE-DEFINITION F GES AM-PH FCC MAGNETIC -3 .28 !

$
$DEFAULT_COMMANDS:
DEFAULT-COMMAND DEF_ELEMENT VA !
DEFAULT-COMMAND REJ_SYS-CONST LIQUID 1 VA !

$DATABASE_INFORMATION:
DATABASE-INFO The following binary and ternary systems are available: '
    FE-CR-NI by Hertzman'
    FE-MO      Fernandez'
    FE-CR-C    Andersson'
    FE-W-C     Gustafson'
    FE-W       Andersson & Gustafson' !

```

Example 2: A Custom Database for the Sb-Sn Binary System

```

$
$ELEMENT, NAME, REF.STATE, ATOMIC-MASS, H0, S0 !
ELEM VA VACUUM          0.0   0.0 0.0 !
ELEM MG HCP(A3)         24.305 0.0 0.0 !
ELEM SB RHOMBOHEDRAL(A7) 121.75 0.0 0.0 !
ELEM SN BCT(A5)         118.69 0.0 0.0 !
ELEM /- ELECTRON-GAS     0      0   0 !

$

```

```

$SPECIES, NAME, STOICHIOMETRIC-FORMULA !
SPECIE MG1 MG1!
SPECIE MG2 MG2!
SPECIE MG2+ MG/+2!
SPECIE SB1 SB1!
SPECIE SB2 SB2!
SPECIE SB4 SB4!
SPECIE SB3- SB/-3!
SPECIE SB5- SB/-5!
SPECIE SN1 SN1!
SPECIE SN4- SN/-4!

$
$PHASE, NAME, TYPE, NR-OF-SUBL, SITES-IN-EACH-SUBL. !
PHASE BCT      Z 1 1.0!
PHASE HCP      Z 1 1.0!
PHASE RHOMBO   Z 1 1.0!
PHASE GAS:G    Z 1 1.0!
PHASE LIQUID:L Z 1 1.0!
PHASE IONICLIQ:Y Z 2 1 1!
PHASE SPLIQ:Y  Z 2 1 1!
PHASE BMG3SB2:I Z 2 3 2!
PHASE AMG3SB2:I Z 2 3 2!
PHASE MG2SN:I  Z 2 2 1!
PHASE SBSN     Z 2 1 1!
PHASE SB2SN3   Z 2 2 3!

$
$CONSTITUENT, PHASE-NAME : CONSTITUENTS !
CONSTITUENT RHOMBO :SB SN:!
CONSTITUENT HCP :MG SN:!
CONSTITUENT BCT :SB SN:!
CONSTITUENT GAS:G :MG1 MG2 SB1 SB2 SB4 SN1:
    > Gas phase, using the Ideal EOS and Mixing Model. !
CONSTITUENT LIQUID:L :SB SN:!
CONSTITUENT IONICLIQ:Y :MG2+:SB SB3- SN SN4- VA:
    > This is the Ionic Liquid Solution Phase. !
CONSTITUENT SPLIQ:Y :MG2+:SB SB3- SN SN4- VA:!
CONSTITUENT BMG3SB2:I :MG2+:SB3- SB5- VA SN4-:!
```

```

CONSTITUENT AMG3SB2:I :MG2+:SB3- VA SN4-:!  

CONSTITUENT MG2SN:I :MG2+ VA:SB3- SN4-:!  

CONSTITUENT SBSN :SB SN:SB SN:!  

CONSTITUENT SB2SN3 :SB:SN:!  

$  

$DEFAULT_COMMANDS:  

DEFAULT-COM DEF-ELEM VA /-!  

DEFAULT-COM REJ-PHASE LIQUID!  

DEFAULT-COM REJ-PHASE SPLIQ!  

$  

$TYPE_DEFINITIONS:  

TYPE-DEFINITION Z SEQ * !  

$  

$DATABASE_INFORMATION:  

DATABASE_INFO The Sb-Sn system with isentropic temperatures!  

$  

$VERSION_DATE:  

VERSION_DATE Last update 1986-05-18 11:39:49 !  

$  

$  

$ HERE COMES THE THERMODYNAMIC DATA (expressed in functions & parameters):  

$  

FUNCTION MGLIQUID 298.15 -4630.90976+192.994374*T-34.0888057*T*LOG(T)  

    -36544605.6*T**(-2); 6000 N!  

$  

FUNCTION MGSOLID 298.15 -8367.34+143.677876*T-26.1849785*T*LOG(T)  

    +4.858E-4*T**2-1.393669E-6*T**3+78950*T**(-1);  

    923.00 Y -13804.4772 +202.909445*T-34.0888057*T*LOG(T)  

    -3.65446056E7*T**(-2) +1.06753982E28*T**(-9); 6000 N!  

$  

FUNCTION SBLIQUID 298.15 9071.98+146.800*T-31.38*T*LOG(T)  

    -2.441646E8*T**(-2); 6000 N!  

$  

.....  

..... <more>  

$  

FUNCTION LFCT 298.15 -17325.6+5.03600*T; 6000 N!

```

```

FUNCTION GFCTSBSN 298.15 LFCT+SBSOLID+SNSOLID+2948.291+3721.286;
    6000 N!

FUNCTION ISB 298.15 15000; 6000 N!

FUNCTION ISN 298.15 47199.9-95.6270*T; 6000 N!

$
.....
..... <more>
$

PARAMETER G(RHOMBO,SB;0) 298.15 SBSOLID; 6000 N!
PARAMETER G(RHOMBO,SN;0) 298.15 2035+SNSOLID; 6000 N!

$

PARAMETER G(HCP,MG;0) 298.15 MGSOLID; 6000 N!
PARAMETER G(HCP,SN;0) 298.15 32000+SNSOLID; 6000 N!
PARAMETER G(HCP,MG,SN;0) 298.15 -69566-9.23183*T; 6000 N!

$

PARAMETER G(BCT,SN;0) 298.15 SNSOLID; 6000 N!
PARAMETER G(BCT,SB;0) 298.15 1000+SBSOLID; 6000 N!
PARAMETER G(BCT,SB,SN;0) 298.15 0.5*ISB+0.5*ISN; 6000 N!
PARAMETER G(BCT,SB,SN;1) 298.15 0.5*ISB-0.5*ISN; 6000 N!

$

PARAMETER G(IONICLIQ,MG2+:SB3-;0) 298.15 -204389-4.98506*T
    -2.75637E9*T**(-2)+3*MGLIQUID+2*SBLIQUID; 6000 N!
PARAMETER G(IONICLIQ,MG2+:SN4-;0) 298.15 -98639.5+881.073*T
    -174.523*T*LOG(T)-1.79808E9*T**(-2); 6000 N!
PARAMETER G(IONICLIQ,MG2+:SB;0) 298.15 SBLIQUID; 6000 N!

$
.....
..... <more>
$

```

Example 3: A Public Database for the Fe-Cr-C Ternary System

```

$
$   Revision history:
$       Created as PDEMO   by Pingfang Shi   on 2004-10-05
$       Renamed to DFeCrC by Pingfang Shi   on 2006-10-25

```

```

TCS Demo Fe-Cr-C Alloy Solutions Database'
(only for demonstration purposes in TCC-Demo/TCW-Demo)'
***** '
      (Version 1.2, Oct. 2006) ''
      Copyright © 2004-2012: Thermo-Calc Software AB, Sweden ''
The DFeCrC database (previously called PDEMO) is the TCS Demo Fe-Cr-C '
Alloy Solutions Database, which is especially designed for primarily '
demonstrating the uses of: '
* TCC-Demo software: BIN, TERN, SCHEIL and some other modules; '
* TCW-Demo software: '
    "Binary" module calculations of phase diagrams and property diagrams'
        in available binary systems; '
    "Ternary" module calculations of phase diagrams (e.g., isothermal'
        sections, monovariant lines involving liquid, liquidus'
        surface projections) and property diagrams in available'
        ternary systems; '
    "Scheil" module simulations of alloy solidifications; and/or '
    "Equilibrium" calculation routines for phase diagrams and property'
        diagrams in available binary or ternary systems. '
It can also be used for other types of calculations/simulations in both'
TCC and TCW software, and in their application programming interfaces.''
It includes critically-assessed data for all possible three binary joins'
(i.e. Cr-C, Fe-Cr and Fe-Cr) and one complete ternary alloy solutions '
within the Fe-Cr-C system. However, due to the fact that experimental'
data for the Fe-C and Cr-C binary joins and Fe-Cr-C ternary system at '
extremely-high temperatures are not sufficient, the available assessed'
data can not be applied to temperature conditions higher than 4000 K.''
Included thermodynamic data are available for various stoichiometric '
and solution phases, e.g. liquid mixture, various alloy solutions and '
intermetallic phases. But the gaseous mixture phase is excluded in this'
DEMO version.''
The DFeCrC database can be used not only in calculating various types '
of phase diagrams (binary phase diagrams, ternary isothermal sections,'
ternary monovariant lines involving liquid, ternary liquidus surface '
projections, ternary isopleth sections, etc.) and property diagrams '
(the easiest ways are through the BIN and TERN modules), but also in '
simulating alloy solidification processes (with the SCHEIL module) of'

```

```

-3.6751551E-21*T**7; 1811 Y
-10839.7+291.302*T-46*T*LN(T); 6000 N!
FUNCT GFEFCC 298.15 +GHSEFE#-1462.4+8.282*T
-1.15*T*LN(T)+6.4E-04*T**2; 1811 Y
-27098.266+300.25256*T-46*T*LN(T)+2.78854E+31*T**(-9); 6000 N!
FUNCT GFECM 298.15 +GPCM1#-10745+706.04*T-120.6*T*LN(T); 6000 N!
FUNCT GFEM23C6 298.15 +7.666667*GFECM#-1.666667*GHSECC#
+66920-40*T; 6000 N!

FUNCT GCRFCC 298.15 +GHSECCR#+7284+.163*T; 6000 N!
FUNCT GCRM23C6 298.15 -521983+3622.24*T-620.965*T*LN(T)
-.126431*T**2; 6000 N!
FUNCT GCRM3C2 298.15 -100823.8+530.66989*T-89.6694*T*LN(T)
-.0301188*T**2; 6000 N!
FUNCT GCRM7C3 298.15 -201690+1103.128*T-190.177*T*LN(T)
-.0578207*T**2; 6000 N!

FUNCT GPCLIQ 298.15 +YCLIQ#*EXP(ZCLIQ#); 6000 N!
FUNCT ACLIQ 298.15 +2.32E-05*T+2.85E-09*T**2; 6000 N!
FUNCT BCLIQ 298.15 +1+3.2E-10*P; 6000 N!
FUNCT CCLIQ 298.15 1.6E-10; 6000 N!
FUNCT DCLIQ 298.15 +1*LN(BCLIQ#); 6000 N!
FUNCT ECLIQ 298.15 +1*LN(CCLIQ#); 6000 N!
FUNCT VCLIQ 298.15 +7.626E-06*EXP(ACLIQ#); 6000 N!
FUNCT XCLIQ 298.15 +1*EXP(.5*DCLIQ#)-1; 6000 N!
FUNCT YCLIQ 298.15 +VCLIQ#*EXP(-ECLIQ#); 6000 N!
FUNCT ZCLIQ 298.15 +1*LN(XCLIQ#); 6000 N!

FUNCT GPCGRA 298.15 +YCGRA#*EXP(ZCGRA#); 6000 N!
FUNCT ACGRA 298.15 +2.32E-05*T+2.85E-09*T**2; 6000 N!
FUNCT BCGRA 298.15 +1+3.6E-10*P; 6000 N!
FUNCT CCGRA 298.15 3.3E-10; 6000 N!
FUNCT DCGRA 298.15 +1*LN(BCGRA#); 6000 N!
FUNCT ECGRA 298.15 +1*LN(CCGRA#); 6000 N!
FUNCT VCGRA 298.15 +5.259E-06*EXP(ACGRA#); 6000 N!
FUNCT XCGRA 298.15 +1*EXP(.9166667*DCGRA#)-1; 6000 N!
FUNCT YCGRA 298.15 +VCGRA#*EXP(-ECGRA#); 6000 N!

```

| | | |
|---------------|------------------------------------------------|---------|
| FUNCT ZCGRA | 298.15 +1*LN(XCGRA#); | 6000 N! |
| FUNCT GPCFCC | 298.15 +YCFCC#*EXP(ZFEFCC#); | 6000 N! |
| FUNCT ACFCC | 298.15 +1.44E-04*T; | 6000 N! |
| FUNCT VCFCC | 298.15 +1.031E-05*EXP(ACFCC#); | 6000 N! |
| FUNCT YCFCC | 298.15 +VCFCC#*EXP(-EFEFCC#); | 6000 N! |
| FUNCT GPCRLIQ | 298.15 +YCRLIQ#*EXP(ZCRLIQ#); | 6000 N! |
| FUNCT ACRLIQ | 298.15 +1.7E-05*T+9.2E-09*T**2; | 6000 N! |
| FUNCT BCRLIQ | 298.15 +1+4.65E-11*P; | 6000 N! |
| FUNCT CCRLIQ | 298.15 3.72E-11; | 6000 N! |
| FUNCT DCRLIQ | 298.15 +1*LN(BCRLIQ#); | 6000 N! |
| FUNCT ECRLIQ | 298.15 +1*LN(CCRLIQ#); | 6000 N! |
| FUNCT VCRLIQ | 298.15 +7.653E-06*EXP(ACRLIQ#); | 6000 N! |
| FUNCT XCRLIQ | 298.15 +1*EXP(.8*DCRLIQ#)-1; | 6000 N! |
| FUNCT YCRLIQ | 298.15 +VCRLIQ#*EXP(-ECRLIQ#); | 6000 N! |
| FUNCT ZCRLIQ | 298.15 +1*LN(XCRLIQ#); | 6000 N! |
| FUNCT GPCRBCC | 298.15 +YCRBCC#*EXP(ZCRBCC#); | 6000 N! |
| FUNCT ACRBCC | 298.15 +1.7E-05*T+9.2E-09*T**2; | 6000 N! |
| FUNCT BCRBCC | 298.15 +1+2.6E-11*P; | 6000 N! |
| FUNCT CCRBCC | 298.15 2.08E-11; | 6000 N! |
| FUNCT DCRBCC | 298.15 +1*LN(BCRBCC#); | 6000 N! |
| FUNCT ECRBCC | 298.15 +1*LN(CCRBCC#); | 6000 N! |
| FUNCT VCRBCC | 298.15 +7.188E-06*EXP(ACRBCC#); | 6000 N! |
| FUNCT XCRBCC | 298.15 +1*EXP(.8*DCRBCC#)-1; | 6000 N! |
| FUNCT YCRBCC | 298.15 +VCRBCC#*EXP(-ECRBCC#); | 6000 N! |
| FUNCT ZCRBCC | 298.15 +1*LN(XCRBCC#); | 6000 N! |
| FUNCT GPFELIQ | 298.15 +YFELIQ#*EXP(ZFELIQ#); | 6000 N! |
| FUNCT AFELIQ | 298.15 +1.135E-04*T; | 6000 N! |
| FUNCT BFELIQ | 298.15 +1+4.98009787E-12*P+3.20078924E-14*T*P; | 6000 N! |
| FUNCT CFELIQ | 298.15 +4.22534787E-12+2.71569924E-14*T; | 6000 N! |
| FUNCT DFELIQ | 298.15 +1*LN(BFELIQ#); | 6000 N! |
| FUNCT EFELIQ | 298.15 +1*LN(CFELIQ#); | 6000 N! |
| FUNCT VFELIQ | 298.15 +6.46677E-06*EXP(AFELIQ#); | 6000 N! |
| FUNCT XFELIQ | 298.15 +1*EXP(.8484467*DFELIQ#)-1; | 6000 N! |

```

FUNCT YFELIQ 298.15 +VFELIQ#*EXP(-EFELIQ#); 6000 N!
FUNCT ZFELIQ 298.15 +1*LN(XFELIQ#); 6000 N!

FUNCT GPFEFCC 298.15 +YFEFCC#*EXP(ZFEFCC#); 6000 N!
FUNCT AFEFCC 298.15 +7.3097E-05*T; 6000 N!
FUNCT BFEFCC 298.15 +1+3.25236341E-11*P+3.36607808E-16*T*P; 6000 N!
FUNCT CFEFCC 298.15 +2.62285341E-11+2.71455808E-16*T; 6000 N!
FUNCT DFEFCC 298.15 +1*LN(BFEFCC#); 6000 N!
FUNCT EFEFCC 298.15 +1*LN(CFEFCC#); 6000 N!
FUNCT VFEFCC 298.15 +6.688726E-06*EXP(AFEFCC#); 6000 N!
FUNCT XFEFCC 298.15 +1*EXP(.8064454*DFEFCC#)-1; 6000 N!
FUNCT YFEFCC 298.15 +VFEFCC#*EXP(-EFEFCC#); 6000 N!
FUNCT ZFEFCC 298.15 +1*LN(XFEFCC#); 6000 N!

FUNCT GPFEBC 298.15 +YFEBC#*EXP(ZFEBC#); 6000 N!
FUNCT AFEBC 298.15 +2.3987E-05*T+1.2845E-08*T**2; 6000 N!
FUNCT BFEBC 298.15 +1+2.80599565E-11*P+3.06481523E-16*T*P; 6000 N!
FUNCT CFEBC 298.15 +2.20949565E-11+2.41329523E-16*T; 6000 N!
FUNCT DFEBC 298.15 +1*LN(BFEBC#); 6000 N!
FUNCT EFEBC 298.15 +1*LN(CFEBC#); 6000 N!
FUNCT VFEBC 298.15 +7.042095E-06*EXP(AFEBC#); 6000 N!
FUNCT XFEBC 298.15 +1*EXP(.7874195*DFEBC#)-1; 6000 N!
FUNCT YFEBC 298.15 +VFEBC#*EXP(-EFEBC#); 6000 N!
FUNCT ZFEBC 298.15 +1*LN(XFEBC#); 6000 N!

FUNCT GPFEHCP 298.15 +YFEHCP#*EXP(ZFEHCP#); 6000 N!
FUNCT AFEHCP 298.15 +7.3646E-5*T; 6000 N!
FUNCT BFEHCP 298.15 +1+32.5236341E-12*P+3.36607808E-16*P*T; 6000 N!
FUNCT CFEHCP 298.15 +26.2285341E-12+2.71455808E-16*T; 6000 N!
FUNCT DFEHCP 298.15 +LOG(BFEHCP#); 6000 N!
FUNCT EFEHCP 298.15 +LOG(CFEHCP#); 6000 N!
FUNCT VFEHCP 298.15 +6.59121E-6*EXP(AFEHCP#); 6000 N!
FUNCT XFEHCP 298.15 +EXP(0.8064454*DFEHCP#)-1; 6000 N!
FUNCT YFEHCP 298.15 +VFEHCP#*EXP(-1*EFEHCP#); 6000 N!
FUNCT ZFEHCP 298.15 +LOG(XFEHCP#); 6000 N!

FUNCT GPCEM1 298.15 +VCEM1#*P; 6000 N!

```

```

$***** FCC_A1 (Solution) *****
$PHASE FCC_A1 %BC 2 1 1 !
$ Note the C TYPE_DEF for 2nd FCC composition-set (MC) is not necessary
$ for the (Fe,Cr)-C system.
PHASE FCC_A1 %B 2 1 1 !
CONST FCC_A1 : CR,FE%
               : C,VA% : !

PARAM G(FCC_A1,CR:VA;0) 298.15 +GCRFCC#+GPCRBCC#; 6000 N REF0 !
PARAM TC(FCC_A1,CR:VA;0) 298.15 -1109; 6000 N REF0 !
PARAM BMAGN(FCC_A1,CR:VA;0) 298.15 -2.46; 6000 N REF0 !
PARAM G(FCC_A1,FE:VA;0) 298.15 +GFEFCC#+GPFEFCC#; 6000 N REF0 !
PARAM TC(FCC_A1,FE:VA;0) 298.15 -201; 6000 N REF0 !
PARAM BMAGN(FCC_A1,FE:VA;0) 298.15 -2.1; 6000 N REF0 !

PARAM G(FCC_A1,CR:C;0) 298.15 +GHSERCR#+GHSERCC#
                        +1200-1.94*T; 6000 N REF2 !
PARAM G(FCC_A1,FE:C;0) 298.15 +GFEFCC#+GHSERCC#+GPCFCC#
                        +77207-15.877*T; 6000 N REF3 !
PARAM TC(FCC_A1,FE:C;0) 298.15 -201; 6000 N REF3 !
PARAM BMAGN(FCC_A1,FE:C;0) 298.15 -2.1; 6000 N REF3 !

PARAM L(FCC_A1,CR:C,VA;0) 298.15 -11977+6.8194*T; 6000 N REF2 !
PARAM L(FCC_A1,FE:C,VA;0) 298.15 -34671; 6000 N REF3 !
PARAM L(FCC_A1,CR,FE:VA;0) 298.15 +10833-7.477*T; 6000 N REF4 !
PARAM L(FCC_A1,CR,FE:VA;1) 298.15 +1410; 6000 N REF4 !
PARAM L(FCC_A1,CR,FE:C;0) 298.15 -74319+3.2353*T; 6000 N REF2 !

$***** BCC_A2 (Solution) *****
PHASE BCC_A2 %A 2 1 3 !
CONST BCC_A2 : CR%,FE%
               : C,VA% : !

PARAM G(BCC_A2,CR:VA;0) 298.15 +GHSERCR#+GPCRBCC#; 6000 N REF0 !
PARAM TC(BCC_A2,CR:VA;0) 298.15 -311.5; 6000 N REF0 !

```

```

PARAM BMAGN(BCC_A2,CR:VA;0) 298.15 -.01; 6000 N REF0 !
PARAM G(BCC_A2,FE:VA;0) 298.15 +GHSEFE# +GPFEBC#; 6000 N REF0 !
PARAM TC(BCC_A2,FE:VA;0) 298.15 1043; 6000 N REF0 !
PARAM BMAGN(BCC_A2,FE:VA;0) 298.15 2.22; 6000 N REF0 !

PARAM G(BCC_A2,CR:C;0) 298.15 +GHSECR# +3*GHSECC# +GPCRBCC# +3*GPCGRA#
                                +416000; 6000 N REF1 !
PARAM TC(BCC_A2,CR:C;0) 298.15 -311.5; 6000 N REF1 !
PARAM BMAGN(BCC_A2,CR:C;0) 298.15 -.008; 6000 N REF1 !
PARAM G(BCC_A2,FE:C;0) 298.15 +GHSEFE# +3*GHSECC# +GPFEBC# +3*GPCGRA#
                                +322050 +75.667*T; 6000 N REF3 !
PARAM TC(BCC_A2,FE:C;0) 298.15 1043; 6000 N REF3 !
PARAM BMAGN(BCC_A2,FE:C;0) 298.15 2.22; 6000 N REF3 !

$ PF-20061025: Modify the L(BCC_A2,FE:C,VA;0) [and L(BCC_A2,CR:C,VA;0)]
$      parametera, in order to avoid BCC-appearance (Fe-C)
$      at temperatures higher than 3900 K.
$PARAM L(BCC_A2,CR:C,VA;0) 298.15 -190*T; 6000 N REF1 !
PARAM L(BCC_A2,CR:C,VA;0) 298.15 -190*T; 3000 Y 0; 6000 N REFS !
$PARAM L(BCC_A2,FE:C,VA;0) 298.15 -190*T; 6000 N REF3 !
PARAM L(BCC_A2,FE:C,VA;0) 298.15 -190*T; 3900 Y 0; 6000 N REFS !
$
PARAM L(BCC_A2,CR,FE:VA;0) 298.15 +20500 -9.68*T; 6000 N REF4 !
PARAM TC(BCC_A2,CR,FE:VA;0) 298.15 1650; 6000 N REF4 !
PARAM TC(BCC_A2,CR,FE:VA;1) 298.15 550; 6000 N REF4 !
PARAM BMAGN(BCC_A2,CR,FE:VA;0) 298.15 -.85; 6000 N REF4 !

PARAM L(BCC_A2,CR,FE:C;0) 298.15 -1250000 +667.7*T; 6000 N REF2 !
PARAM TC(BCC_A2,CR,FE:C;0) 298.15 1650; 6000 N REF5 !
PARAM TC(BCC_A2,CR,FE:C;1) 298.15 550; 6000 N REF5 !
PARAM BMAGN(BCC_A2,CR,FE:C;0) 298.15 -.85; 6000 N REF5 !

$***** HCP_A3 (Solution) *****
$PHASE HCP_A3 %BC 2 1 .5 !
$ Note the C TYPE_DEF for 2nd HCP composition-set (M2C) is not necessary
$ for the (Fe,Cr)-C system.
PHASE HCP_A3 %B 2 1 .5 !

```

```

CONST HCP_A3 : CR,FE,
              : VA%,C : !

PARAM G(HCP_A3,CR:VA;0) 298.15 +GHSERCR#+4438; 6000 N REF1 !
PARAM TC(HCP_A3,CR:VA;0) 298.15 -1109; 6000 N REF1 !
PARAM BMAGN(HCP_A3,CR:VA;0) 298.15 -2.46; 6000 N REF1 !
PARAM G(HCP_A3,FE:VA;0) 298.15 +GHSEFFE#+GPFHCP#
                        -3705.78+12.591*T-1.15*T*LN(T)+6.4E-04*T**2; 1811 Y
                        +GHSEFFE#+GPFHCP#
                        -3957.199+5.24951*T+4.9251E+30*T**(-9); 6000 N REF0 !
PARAM G(HCP_A3,CR:C;0) 298.15 +GHSERCR#+.5*GHSEGCC#
                        -18504+9.4173*T-2.4997*T*LN(T)+.001386*T**2; 6000 N REF1 !
PARAM G(HCP_A3,FE:C;0) 298.15 +GFEFCC#+.5*GHSEGCC#+GPCFCC#
                        +52905-11.9075*T; 6000 N REF3 !

PARAM L(HCP_A3,CR:C,VA;0) 298.15 +4165; 6000 N REF1 !
PARAM L(HCP_A3,FE:C,VA;0) 298.15 -22126; 6000 N REF3 !
$PARAM L(HCP_A3,FE:C,VA;0) 298.15 -17335; 6000 N TCFE3 !
PARAM L(HCP_A3,CR,FE:VA;0) 298.15 +10833-7.477*T; 6000 N REF4 !

$***** SIGMA (Solution) *****
PHASE SIGMA % 3 8 4 18 !
CONST SIGMA : FE
              : CR
              : CR,FE : !

PARAM G(SIGMA,FE:CR:CR;0) 298.15 +8*GFEFCC#+22*GHSERCR#
                        +92300-95.96*T+GPSIG1#; 6000 N REF4 !
PARAM G(SIGMA,FE:CR:FE;0) 298.15 +8*GFEFCC#+4*GHSERCR#+18*GHSEFFE#
                        +117300-95.96*T+GPSIG2#; 6000 N REF4 !

$***** CEMENTITE (Solution) *****
PHASE CEMENTITE % 2 3 1 !
CONST CEMENTITE : CR,FE%
                  : C : !

PARAM G(CEMENTITE,CR:C;0) 298.15 +3*GHSERCR#+GHSEGCC#

```

```

-48000-9.2888*T; 6000 N REF2 !

PARAM G(CEMENTITE,FE:C;0) 298.15 +GFECCEM#; 6000 N REF3 !

PARAM L(CEMENTITE,CR,FE:C;0) 298.15 +25278-17.5*T; 6000 N REF2 !

$***** M3C2 (Compound) *****
PHASE M3C2 % 2 3 2 !
CONST M3C2 : CR
           : C : !

PARAM G(M3C2,CR:C;0) 298.15 +GCRM3C2#; 6000 N REF2 !

$***** M7C3 (Solution) *****
PHASE M7C3 % 2 7 3 !
CONST M7C3 : CR%,FE
           : C : !

PARAM G(M7C3,CR:C;0) 298.15 +GCRM7C3#; 6000 N REF2 !
PARAM G(M7C3,FE:C;0) 298.15 +7*GHSEFE#+3*GHSECC#
                    +75000-48.2168*T; 6000 N REF2 !

PARAM L(M7C3,CR,FE:C;0) 298.15 -4520-10*T; 6000 N REF2 !

$***** M23C6 (Solution) *****
PHASE M23C6 % 3 20 3 6 !
CONST M23C6 : CR%,FE%
            : CR%,FE%
            : C : !

PARAM G(M23C6,CR:CR:C;0) 298.15 +GCRM23C6#; 6000 N REF5 !
PARAM G(M23C6,FE:CR:C;0) 298.15 +.1304348*GCRM23C6#
                    +.8695652*GFEM23C6#; 6000 N REF5 !
PARAM G(M23C6,CR:FE:C;0) 298.15 +.8695652*GCRM23C6#
                    +.1304348*GFEM23C6#; 6000 N REF5 !
PARAM G(M23C6,FE:FE:C;0) 298.15 +GFEM23C6#; 6000 N REF5 !

PARAM L(M23C6,CR,FE:CR:C;0) 298.15 -205342+141.6667*T; 6000 N REF2 !

```

PARAM L(M23C6,CR,FE:FE:C;0) 298.15 -205342+141.6667*T; 6000 N REF2 !

\$***** GRAPHITE (Compound) *****

PHASE GRAPHITE % 1 1.0 !

CONST GRAPHITE : C : !

PARAM G(GRAPHITE,C;0) 298.15 +GHSECC#+GPCGRA#; 6000 N REF0 !

\$

\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$

\$ ASSESSED_SYSTEMS information:

\$ * necessary for the BIN and TERN modules in TCC

\$ the Binary Phase Diagram module in TCW

\$ and the Equilibrium calculation routine in TCW

\$-----

ASSESSED_SYSTEM

\$... Binary ...

C-FE(;P3 TMM:300/4000 *)

C-CR(;P3 TMM:300/4000 *)

CR-FE(;G5 MAJ:BCC/FE:VA C_S:BCC/CR:VA

;P3 TMM:300/3000 STP:.6/1200/1/-2/2)

\$ CR-FE(TDB -HCP ;G5 MAJ:BCC/FE:VA C_S:BCC/CR:VA

\$;P3 TMM:300/3000 STP:.6/1200/1/-2/2)

\$

\$... Ternary ...

C-CR-FE(;G5 MAJ:BCC/FE:VA C_S:BCC/CR:VA

;P3 STP:.4/.5/1 STP:0.1/0.5/1)

!

\$

\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$\$

\$

\$ LIST OF REFERENCE:

\$

\$-----

LIST_OF_REFERENCES

NUMBER SOURCE

REF0 'Alan Dinsdale, SGTE Data for Pure Elements, Calphad Vol 15(1991)
p 317-425, also in NPL Report DMA(A)195 Rev. August 1990'

REF1 'J-O Andersson, Calphad Vol 11 (1987) p 271-276, TRITA 0314; C-CR'

REF2 'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'

REF3 'P. Gustafson, Scan. J. Metall. vol 14, (1985) p 259-267
TRITA 0237 (1984); C-FE'

REF4 'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92
TRITA 0270 (1986); CR-FE'

REF5 'J-O Andersson, Met. Trans A, Vol 19A, (1988) p 627-636
TRITA 0207 (1986); C-CR-FE'

REFS 'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys Database,
v1.2; Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters
at high temperatures.'

!

The Database Checker

In this section:

| | |
|-----------------------------------------|----|
| About the Database Checker | 68 |
| Database Checker Revision History | 69 |

About the Database Checker

The Thermo-Calc software package includes a program to check that the syntax of unencrypted database files is correct. The program applies the syntax rules set out in the *Database Manager User Guide* and reports errors and issues warnings. This program is intended for advanced users who develop and manage databases.



Thermo-Calc accepts deviations from these syntax rules. This means that a database can work even if the Database Checker reports errors and warnings. For example, an error is reported if an abbreviated phase name is found, but phase name abbreviations are accepted by Thermo-Calc and its add-on modules.

The executable **DatabaseChecker** file is found in the Thermo-Calc home directory. The program can also be launched by selecting **Tools → Database Checker** from the main menu.



["Database Checker Revision History" on the next page](#) for releases notes that may assist database developers.

Custom Databases: GES5 and GES6 Calculation Engine Version

As of Thermo-Calc version 2019b, the default calculation engine is set to GES6. For custom database users, you may sometimes see messages in the log indicating that additional preparation is being done by Thermo-Calc prior to a calculation. The preparation is carried out automatically; it is usually fast and only needed the first time a custom database is used after a modification. While databases with warnings are tolerated, databases that contain errors can only be loaded by GES6 after the errors are corrected.

The Database Checker tool uses the same parser as GES6 and can be used to verify the consistency and correctness of databases during development, before the databases are actually used.



["Database Checker" on page 35](#)



To globally set the default from GES6 back to GES5, go to the **Tools → Options → "General" on page 37** tab and click **Version 5** for the *Preferred Gibbs Energy System* setting. The ["SET GES VERSION" on page 118](#) Console Mode command is used to change GES versions for a single Thermo-Calc session.



Contact Thermo-Calc Software AB at info@thermocalc.com for more information about the changes or if you encounter any issues you think are related to the new version of the calculation engine.

Database Checker Revision History

The DatabaseChecker application is standalone and need not be installed separately, just download the containing zip file, open it and follow the instructions in the README.TXT file. The program requires that Java is installed on the target machine. Please note that large amounts of RAM may be required when checking large databases.

RELEASE NOTES VERSION 1.4

- The DatabaseChecker user interface has been modified to allow checking of several database files in one batch. Instead of selecting an individual database file, the user now selects a directory that contains databases. The application then shows a tree structure with all database files in the chosen directory and its subdirectories. The user may then select any number of these files for processing.
- A check of parameters whose interaction order is 3 has been introduced. For such parameters, there must either exist one parameter with the interaction degree 0 or three parameters with the interaction degrees 0, 1 and 2.
- To facilitate optimization of databases, the tool now generates information messages about functions and parameters that will always return 0.

RELEASE NOTES, VERSION 1.3.2

- The tool now detects conflicts between identical parameters even if one of them have been defined with the G prefix and the other with the L prefix.

RELEASE NOTES, VERSION 1.3

A bug prevented integers bigger than 32 bits from being parsed. This has been corrected.

The tool now checks that the species and number of sublattices used in parameter definitions match the phase definition and generates an error message for every mismatch. Ionic liquid parameters are currently exempted from this check as not to break the widespread use of defining only one constituent for ionic liquid parameters.

Type definitions and case statements are now parsed for errors. However, only a subset of all possible GES, POLY and TDB commands are accepted and all other commands will result in an error message. The accepted commands are:

- GES AMEND_PHASE_DESCRIPTION
- COMPOSITION_SETS
- MAJOR_CONSTITUENTS
- DISORDERED_PART
- MAGNETIC_ORDERING
- STATUS_BITS
- DEFAULT_STABLE
- FRACTION_LIMITS
- EXCESS_MODEL
- REDLICH-KISTER_MUGGIANU
- HKF
- HKF_ELECTROSTATIC
- DEBYE_HUCKEL
- GES CHANGE_STATUS
- TDB DEFINE_SYSTEM_ELEMENTS
- TDB RESTORE_PHASES
- TDB REJECT_PHASES

Some improvements to warning and error messages have been made to facilitate finding errors.

RELEASE NOTES, VERSION 1.2

- The tool now uses parallel processing of database files on multi-core systems. This significantly improves performance when large databases are checked.
- It is no longer required that inter-dependent database statements are defined in a specific order in the database file (e.g., species need not any longer be defined before the elements on which they depend). However, for the sake of readability, it is still advised that the database statements occur in a natural order in the file.
- Because of the parallel processing of database statements, multiple definition errors (cases where one name has been used to define more than one entity in the

database e.g, two identically named species) may now be generated for any of the violating occurrences and not only for the last occurrence in the file.

RELEASE NOTES, VERSION 1.1

- Phase names were not properly recognized in parameter definitions if there was one or more whitespace characters between the opening parenthesis and the phase name. This has been corrected.
- The error message Could not parse parameter, <species name> has been given without a sublattice number but is defined in more than one sublattice is now displayed only for phases where the general diffusion model is used. Note: this implementation is temporary and may be subject to changes later.
- The meaning of the information message The phase <phase name> expects the following parameters: [<parameter names>] was unclear to users. It is now longer shown for the parameter names T and P. For all other names, the message is now displayed as an error message with the following text: The phase <phase name> contains references to the following undefined functions: [<function names>].
- The tool now looks for function names that are abbreviations of other function names and warns about this, since abbreviated names may cause problems during the execution of macro files that have been auto-generated from GES.
- The tools also warns for functions whose names are in the format V<integer>, since this may cause conflicts with names that are used by PARROT.
- Parameter names are now shown in a format that is less cryptic and more resembles the format used in the database. However, the format of diffusion parameters may still differ somewhat from what is used in the database.

RELEASE NOTES, VERSION 1.0

- The tool parses a TDB file and produces a log with error, warning and information messages about the state of the file
- The message log can be exported and saved as a separate file for later analysis
- The tool is based on the database command definitions given in TC_Database_ManagersGuide and DICTRA27_UsersGuide. All commands in these documents are supported. Some undocumented DIFFUSION commands are not supported.
- Databases that span several files are correctly handled, also blocked files
- The tool is in some aspects more strict than required by the guides (see Additional Information below)

-
- The tool performs the following checks:
 - Syntax control of database statements: ERROR
 - Line size: ERROR or WARNING depending on context
 - Multiply defined elements, species or phases: ERROR
 - Multiply defined functions and parameters: ERROR
 - Multiply defined assessed system: ERROR
 - Multiply defined references: ERROR
 - References entries that are never used: WARNING
 - References to non-existent type definitions: ERROR
 - Type definitions that are never used: WARNING
 - Unused functions and parameters: WARNING
 - Functions and parameters with undefined references: WARNING
 - References to undefined elements, species or phases: ERROR
 - Dependencies to external names from a phase: INFORMATION. (All parameters of a phase are evaluated with respect to their dependencies to other parameters and functions and all unresolved names are listed. Typically, this should only yield dependencies on T and possibly P)

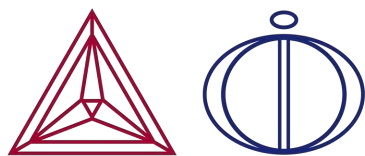
ADDITIONAL INFORMATION

In addition to the command definitions given in the user guides listed above, the following rules are also applied:

- Names are case-sensitive, meaning that e.g., the defined element MN cannot be referred to under the name Mn;
- Phase names cannot be abbreviated. When referred to in parameter descriptions their full names must be used.

DATAPLOT User Guide

Thermo-Calc Version 2020a



Introduction to the DATAPLOT User Guide

In this section:

| | |
|---------------------------------------------|---|
| Using this Guide | 3 |
| About the DATAPLOT Graphical Language | 3 |
| Plotting Experimental Data Files | 4 |

Using this Guide

The *DATAPLOT User Guide* gives all the details on the graphical language DATAPLOT that a phase diagram or property diagram calculated by Thermo-Calc or a kinetic profile simulated by the Diffusion Module (DICTRA) can be defined.

This guide

- Discusses the important features of the DATAPLOT language.
- Describes the commands to define PROLOGUE and DATASET.
- Several examples and the standard codes for formatting are provided.

One topic introduces the method of formatting DIGLIB symbols in LaTeX documents, for the purpose of necessarily/appropriately referring to the corresponding LaTeX symbols (closest to those DIGLIB symbols which have been plotted on a diagram using the DATAPLOT Graphical Language) in the texts of LaTeX documents for publications/reports.

About the DATAPLOT Graphical Language

In order to obtain graphical output of any numerical data and informative strings, a graphical language called DATAPLOT was developed in connection with the graphical software DIGLIB. Using this graphical language, you can store information in a normal text file (*.EXP), which can be plotted as graphical symbols, lines, texts or Greek letters on any plot device support by DIGLIB.

You can generate and plot DATAPLOT (*.EXP) files together with various calculation and/or experimental results from, for example, phase and property diagrams calculated with the Thermo-Calc software composition profiles or other diagrams simulated by the Diffusion Module (DICTRA).

An EXP file automatically generated by the POST-processor (using the ["MAKE_EXPERIMENTAL_DATAFILE" on page 360](#) command) in the Thermo-Calc software is a DATAPLOT (*.EXP) file and may contain all types of legal DATAPLOT commands and parameters. With a text editor, you can modify or add some DATAPLOT commands and related parameters in an existing EXP file. This is useful when appending experimental information to calculated/simulated plots, and when specifying user-defined texts, symbols, colors, fonts, filled patterns, diagram types, diagram sizes, symbol/character sizes, titles, special characters, etc.



There is another type of experimental data file that is generated in Thermo-Calc when working with the PARROT module. For more information see ["Experimental Data Files \(*.POP, *.DOP\)" on page 31](#).

DATAPLOT Examples

To help you prepare your EXP (experimental) files to use for your plotted diagrams generated by Thermo-Calc simulations, there are examples of EXP files using the DATAPLOT graphical language standard, which are normally independent of software versions.


Plotting Experimental Data Files



You can read and plot experimental data files in both Console Mode and Graphical Mode.

Graphical Mode

In Graphical Mode, the Experimental File Reader activity can only be created from the top My Project node. This activity allows you to read an experimental data file (*.EXP). This type of file has information specifying a plotted diagram, written in the DATAPLOT graphical language. From this activity node you can plot the EXP file or save a copy of the file to another location.

PLOTTING AN EXP FILE WITH THE EXPERIMENTAL FILE READER

1. Right-click **My Project** and from the **Create New Activity** submenu choose **Experimental File Reader**.
2. In the **Configuration** window in the **EXP file** field, enter the name of the EXP file to plot. Or click the **Select Exp file**  button to navigate to a location on the computer.
3. Right-click the **Experimental File Reader** node and from the **Create New Successor** submenu choose **Plot Renderer**.

If the source EXP file is changed, you can also click the **Reload the selected EXP file from disk**  button to refresh the data. If you want to save or export the loaded file, click the **Save EXP file**  button, then navigate to where you want to save it and give it a file name.

4. In the **Configuration** window click **Perform** or right-click the **Plot Renderer** node and select **Perform**.

Console Mode

In Console Mode you use the QUICK EXPERIMENTAL PLOT command found in the POLY-3 POST module (as well as in the Diffusion Module (DICTRA) POST module) to plot the .EXP files. This command can be used when there is no graphical information to be plotted in the

POLY3 workspace. It defines a pair of axes, sets the axis labels to X and Y, and scales both X- and Y-axes between 0.0 and 1.0 unless a prologue is read from the DATAPLOT (*.EXP) data file.

PLOTTING AN EXP FILE IN THE POST MODULE

1. Go to the POLY-3 Module: At the SYS prompt type `Go Poly`.
2. Go to the POST module: At the POLY_3 prompt type `Post`.
3. At the POST prompt, type `Quick`.
4. Enter Prologue and Dataset numbers (if applicable). See ["QUICK EXPERIMENTAL PLOT" on page 362](#).
5. AT the POST prompt, type `Plot`.

Using DATAPLOT Graphical Language

In this section:

| | |
|----------------------------------------------------|----|
| DATAPLOT File Structure | 7 |
| DATAPLOT Language Syntax | 7 |
| Coordinate Systems | 7 |
| Graphical Operation Codes | 8 |
| Tables or Blocks | 9 |
| Drawing a Polygon | 10 |
| Drawing an Analytical Function | 10 |
| Painting of an Enclosed Area | 10 |
| Writing a Text | 11 |
| Plotting a Symbol | 11 |
| Other Commands | 11 |
| Interactive Plotting | 12 |
| Formatting DIGLAB Symbols in LaTeX Documents | 13 |
| LaTeX Formatting Codes | 14 |

DATAPLOT File Structure

A DATAPLOT file is a normal text file with the extension `EXP` that can be created with a text editor or by a program. The file must contain one or more `DATASETS` and possibly also one or more `PROLOGUES`. Each `PROLOGUE/DATASET` is an entity that can be individually selected for plotting.

A `PROLOGUE/DATASET` is identified by a unique positive number in the file. A `PROLOGUE` normally contains various `DATASET` commands for defining information about axis scaling, axis text, axis length, title and so on. A `PROLOGUE` is terminated by another `PROLOGUE` or by the first `DATASET`. This means that all `PROLOGUES` must be placed at the beginning of the file, before the first `DATASET`.

A `DATASET` normally contains `DATASET` commands that are associated to separate data points, as well as with one or more `BLOCKS` of data (calculated or experimental). A `DATASET` is terminated by another `DATASET` command or the end of file.

DATAPLOT Language Syntax

The DATAPLOT language consists of commands with or without parameters:

```
COMMAND {parameter(s)}
```

The basic graphical command consists of an X/Y coordinate pair and a Graphical Operation Code (`GOC`). With other commands, the interpretation of this basic command can be modified. There are separate commands to draw a polygon or a function and ways to get texts in different fonts.

To edit a DATAPLOT file, the graphical commands can be abbreviated.



A command (with parameters) must not exceed 80 characters. If it is too long (normally as writing necessary codes in a command's parameters for a complex expression), two or more lines can be edited.

Coordinate Systems

The DATAPLOT language accepts coordinates in three different coordinate systems, which are called *word*, *virtual* and *normalized*.

- The *word* coordinates are selected to represent any kind of data and be of “any” magnitude.
- The *virtual* coordinate system uses centimeters as units. However, the actual size of one unit is dependent on the implementation of the device driver in DIGLIB. It is not

recommended to use this coordinate system if different output devices are used for preliminary and final plots.

- The *normalized* coordinate system goes from zero to one. When plotting, you interactively scale each axis by selecting the minimum and maximum word coordinates on the axis. In the normalized coordinate system, the minimum axis value is represented by zero and the maximum by one. DIGLIB draws a square between the four points (of the X and Y axes) that are determined by the coordinates zero and one in the normalized coordinates.



It is also possible to draw triangular plots as described below. However, in most places, it only references square diagrams. All data points within the minimum and maximum word coordinates are plotted inside this square. DIGLIB also writes tic marks and corresponding word values at such tic marks.

It may be convenient to use normalized coordinates to draw boxes and texts. You can give normalized coordinates outside zero and one if you want to write texts outside the area enclosed by the square. To ensure proper operation outside the normalized box, the clipping must be turned off.

Graphical Operation Codes

The Graphical Operation Code (GOC) determines how the coordinates are interpreted and what is done at the point determined by the coordinates. For an individual data point, its GOC codes must be given. For each data ["BLOCK" on page 21](#), you define a default GOC that is used for the whole BLOCK, unless a GOC is explicitly defined for a specific point.

- If *s* is omitted, no symbol is plotted. A number selecting the symbol can optionally follow the character *s*. The DIGLIB software determines which symbol the number represents. See ["Plotting a Symbol" on page 11](#).
- If any of the other characters are omitted, the default defined for the BLOCK is used. Absolute values imply the current coordinates; relative values mean that these are added to the current coordinates. The GOC must be written without any space between various characters, but the order for the characters is irrelevant.
- If no GOC is defined for a BLOCK, the system default is MWA, (Move Word Absolute), i.e., move to the given point that is interpreted as absolute word coordinates. GOC=DNA means draw a line from the current point to the new one interpreting the coordinates as normalized. After each draw or move operation, the so-called current point is the new point.
- The ["TEXT" on page 29](#) following the ' command is interpreted and expanded by the DIGLIB software, if it includes any ^ operator or ["STRING" on page 28](#) names using

the ~ descriptor. To get PostScript outputs, the TEXT must be edited by the LaTeX Text Formatting Program instead (see ["LaTeX Formatting Codes" on page 14](#)).

GOC CHARACTER DEFINITIONS

The GOC is a combination of the following characters:

| Character | Meaning |
|-----------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| W, V or N | To use word (W), virtual (V) or normalized (N) coordinates. W is the default. |
| A or R | XY are absolute (A) or relative (R) values. A is the default. |
| M or D | To perform a move (M) or draw (D) operation to XY. M is the default. |
| B | To apply "soft" splines on a line drawn between the coordinate pairs (used only on BLOCK data). |
| S | To plot default symbol at XY. |
| S# | To change default symbol to No # symbol and plot it at XY. |
| `TEXT | To plot TEXT at XY. It must be the last operation in a GOC code. The TEXT following the ' command is interpreted and expanded by the DIGLIB software, if it includes any ^ operator or STRING names using the ~ descriptor. |

Tables or Blocks

In many cases, you have (calculated or experimental) data in the form of tables, and want to plot one or several columns as X-axis and one or more columns as Y-axis. A single table can contain many sets of data records of the same kind of information for a specific data ["BLOCK" on page 21](#). There can be many data BLOCKS in a ["DATASET" on page 24](#).

By enclosing these tables in a data BLOCK, you can select which column(s) is the X-axis and which is the Y-axis. For example,

```
BLOCK X=C1; Y1=C3; Y2=C2; GOC=C4,DAW
```

Where the X-axis values are in column 1, the Y-axis values are in columns 2 and 3, and any GOC codes are in column 4. The default GOC for this BLOCK is Draw Absolute Word. The GOC code inside the table is only necessary if the default GOC is not applicable.

A more elaborate use of the table is shown in this example:

```
BLOCK X=C3; Y=1E3/ (C3+273); GOC=C8,MAWS1
```

Where the X-axis values are in column 3, the Y-axis values are in column 1 with some additional calculations applied. Any GOC is in column 8, and the default GOC is Move Absolute Word and plot the symbol no. 1.

Columns in a table must be separated by one or more space characters and do not have to be justified.

It is possible to have tables with mixed text and numbers, but each word followed by a space is counted as one column. The columns used for plotting also must be numerical. An example of a legal line in a table is

```
298.15 This_is_the_second_column 11.5 This_is_the_fourth_column
```



A line in the table must not exceed 80 characters. A BLOCK must be terminated by a line with the ["BLOCKEND" on page 22](#) command.

Drawing a Polygon

Normally, each point is written on a separate line. But in order to draw a line in a more compact way, use the command ["DRAWLINE" on page 24](#). DRAWLINE is followed by a couple of X/Y number pairs. The X/Y pairs must be separated by a space, and there must be a comma sign between the X and Y values. DRAWLINE makes a move operation to the first pair of X/Y coordinates, and then draws a line among all pairs up to the last one. All pairs must fit on one line of 80 characters, but there can be several consequent DRAWLINE commands.



["Example 2 – Draw Polygons and Symbols" on page 32](#)

Drawing an Analytical Function

Use a ["BLOCK" on page 21](#) command to set an axis to a function. It is not necessary to use a value from any column in order to compute the function value to be plotted. Use the ["FUNCTION" on page 25](#) command to plot a function with an even increment of the independent variable.



["Example 4 – Draw Curves Defined by Functions" on page 36](#)

Painting of an Enclosed Area

Use the ["PAINT" on page 27](#) command to paint or fill an area in a specified pattern in the plot. Available patterns are determined by the DIGLIB software. A related command to PAINT is ["PCFUNCTION" on page 27](#).

Writing a Text

Use the ["TEXT" on page 29](#) command to write a text at the current point. You can write a text at any X/Y pair by appending a single quote followed by the text on the same line. For example:

```
1.1 1.0 NAM'This is a text
```

writes `This is a text` at the normalized coordinates (1.1, 1.0).

Use the command ["FONT" on page 25](#) to select the font used for the text, and ["CHARSIZE" on page 22](#) to select the size of the characters. Set this size of the symbols with ["SYMBOLSIZE" on page 28](#).

If a text or a single character should be of a different font than all the other text, or to use subscripts or superscripts in a text, use the `^` operators or `STRING` command to create the text. The command ["STRING" on page 28](#) stores the text in a specified variable that includes all text-formatting information defined by the DIGLIB software.



["Example 3 – Using Strings and Various Line Types" on page 34](#) and ["Example 5 – Use Included Files for Predefined Symbols" on page 38](#).

However, if a graphical output is done on a PostScript device using the PostScript hardcopy fonts, special text formatting codes as ["LaTeX Formatting Codes" on page 14](#) should be used and the `STRING` formatting syntax is then not valid.

Plotting a Symbol

As described in ["Graphical Operation Codes" on page 8](#), a GOC code in a data BLOCK may contain an `s` option to plot a symbol for an X/Y pair or the same symbols for the data BLOCK. A number selecting the symbol can optionally follow the character `s`. You can plot a symbol at any current X/Y position by appending a quote specified by the symbol number in the GOC code (e.g., `1.1 1.0 MANS5'This is a text`).

You can also insert DIGLIB symbols into LaTeX-edited documents.



["Example 1 – Draw Lines and Symbols" on page 31](#), ["Example 2 – Draw Polygons and Symbols" on page 32](#) and ["Example 8 - DIGLIB Symbols" on page 51](#)

Other Commands

General

- When plotting symbols representing various experimental data, it is important that the symbols are centered around the coordinate values.

-
- The dollar sign \$ as the first character of a line stands for a comment character, which means the whole line is ignored when plotting.

ATTRIBUTE

Use the ["ATTRIBUTE" on page 21](#) command to change the coordinates where text is displayed. The default is the lower left corner of the first character in the text.

CLIP

Use the ["CLIP" on page 22](#) command to change the default where all data outside the normalized coordinates zero and one are not plotted.

COLOR

If you are using a color device, use the ["COLOR" on page 23](#) command to change color of the lines. On some black and white devices, colors are simulated with different width and dashing of the lines.

INCLUDE

Use the ["INCLUDE" on page 26](#) command to create libraries with texts and include these in similar plots.

LINETYPE

Use the ["LINETYPE" on page 26](#) command to define line types as solid, long dashed, short dashed or dotted.

Interactive Plotting

The DATAPLOT file is read into the POST module in the workspace with ["APPEND EXPERIMENTAL_DATA" on page 353](#) or ["QUICK_EXPERIMENTAL_PLOT" on page 362](#). These commands ask for the name of the DATAPLOT file and also which PROLOGUE(S) and DATASET(S) are to be plotted.

See the *Thermo-Calc Command Mode Reference Guide* for details about these commands.

By giving the PROLOGUE/DATASET number as -1, you get a list of the available PROLOGUES/DATASETS in the file. Note that if `DATASET 0` is in a DATAPLOT file, its data is always used even if other DATASETS are chosen.

Formatting DIGLAB Symbols in LaTeX Documents

When using the LaTeX editor, you can use the DIGLIB symbols in texts and in figures. This then refers to the corresponding LaTeX symbols (closest to those DIGLIB symbols which are plotted on a plot using the DATAPLOT Graphical Language) in the texts of LaTeX documents for publications/reports.

This topic shows how to generate some DIGLIB symbols in texts, through the attached LaTeX source file and its converted jpg file.



["Example 8 - DIGLIB Symbols" on page 51](#)

DIGLIB_SYM.TEX

```
\documentclass[dvips,12pt]{article}
\textwidth 165mm
\textheight 225mm
\oddsidemargin 1mm
\evensidemargin 1mm
\topmargin 1mm
%%\usepackage{amssymb}
%% next replace amssymb and to get udtimes
\usepackage[utopia]{mathdesign}
\usepackage{rotating}
\usepackage[latin1]{inputenc}
\usepackage{graphics}
\usepackage{graphicx,subfigure}% with figures
%\usepackage[draft]{graphicx}% without figures
\usepackage{subfigure}% with figures
\topmargin 1mm
\oddsidemargin 1mm
\evensidemargin 1mm
\begin{document}
{\Large \bf Diglib symbols and their corresponding LaTeX symbols}
\vspace{5mm}
```

The information below gives the closest corresponding LaTeX symbol. All symbols (except +) must be generated in math mode. Most of these require the package `amssymb`, i.e., you need a directive `usepackage{amssymb}` in the preamble. Two of the symbols require the more extensive `mathdesign` that can be included with `usepackage[utopia]{mathdesign}`.

```
\vspace{5mm}

{\Large

\begin{tabular}{llll}

Diglib & Latex & Latex name & Note\\

1&  $\vartriangle$ &  $\backslash\vartriangle$  & amssymb \\

2&  $\square$ &  $\backslash\square$ \\

3& {\Huge  $\diamond$ } &  $\backslash\diamond$  & size  $\backslash$Large \\

4&  $\udtimes$ &  $\backslash\udtimes$  & mathdesign \\

5&  $\triangledown$ &  $\backslash\triangledown$  & amssymb\\ 6 & +& normal + \\

7&  $\ast$ &  $\backslash\ast$  & amssymb\\

8&  $\times$ &  $\backslash\times$  \\

9& {\Huge  $\circ$ }&  $\backslash\circ$  & size  $\backslash$Large \\

10& {\Huge  $\star$ }&  $\backslash\star$  & size  $\backslash$Large, amssymb\\

11&  $\curlyvee$ &  $\backslash\curlyvee$  & amssymb\\

12&  $\Join$ &  $\backslash\Join$ \\

13&& - & nothing similar, overlapping  $\rangle \langle$ \\

14&& - & nothing similar, 10-edged star \\

15&  $\maltese$ &  $\backslash\maltese$  & mathdesign \\

16&& - & nothing similar, a pentagon \\

17&  $\curlywedge$ &  $\backslash\curlywedge$  & amssymb\\

\end{tabular}}

\end{document}$$$ 
```

LaTeX Formatting Codes



For a list of supported LaTeX commands, see:

<http://www2.ph.ed.ac.uk/snuggletex/documentation/math-mode.html>.



By default when using the LaTeX command, you are in math mode and Thermo-Calc automatically interprets the entered text as math. The above link uses the dollar sign (\$) in all the examples but this is NOT required. For example, if you enter $E=mc^2$ this is displayed including the \$ instead of the equation.



As of Thermo-Calc 2015a the LTEXT text formatting is replaced by LaTeX. For existing users who may have plots and files that use the LTEXT format, and especially when using Console Mode, the following examples show the command changes from LTEXT and its LaTeX equivalent:

LTEXT vs LaTeX Commands for Labels

| Symbol or text format | LTEXT | LaTeX |
|----------------------------|---------------------------------------------------------------|------------------------------------------------------|
| Subscripts in an axis text | S-A-TEXT Y N Mole-fraction Al ^{DO2} O ^{DO3} | S-A-TEXT Y N \latex Mole-fraction Al _{2O_3} |
| Label with subscript | add .13 .15 n c-ZrO ^{DO2} | add .13 .15 n \latex c-ZrO ₂ |
| Greek symbol | ADD .05 .50 N ^GRd | ADD .05 .50 N \latex \delta |

PROLOGUE Commands

In this section:

| | |
|--------------------|----|
| PROLOG | 17 |
| DIAGRAM_TYPE | 17 |
| TIC_TYPE | 17 |
| TITLE | 17 |
| XLENGTH | 18 |
| XSCALE | 18 |
| XTEXT | 18 |
| XTYPE | 18 |
| YLENGTH | 18 |
| YSCALE | 18 |
| YTEXT | 19 |
| YTYPE | 19 |

PROLOG

PROLOG is the beginning of a number of consequent lines of user-defined diagram layout commands. The lines are displayed with the `optional text` when using the `-1` option in the POST-processor as prompted for the PROLOG number with ["APPEND EXPERIMENTAL DATA" on page 353](#) or ["QUICK_EXPERIMENTAL_PLOT" on page 362](#).



["Examples of DATAPLOT Files and Outputs" on page 30](#)

| Syntax |
|---------------------------------------------------------------|
| <code>PROLOGUE # optional text</code> |
| <code>#</code> is an unsigned integer identifying the PROLOG. |

DIAGRAM_TYPE

DIAGRAM_TYPE sets the diagram type to square (the default) or triangular.



This is available for Console Mode.



["Example 6 – Triangular Diagrams for Ternary Systems" on page 40](#)

| Syntax |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>DIAGRAM_TYPE type plot_3rd_axis clip_along_third-axis</code> |
| <code>type</code> is a character string reading SQUARE (default) or TRIANGULAR. If <code>type</code> reads TRIANGULAR, then two additional parameters are given: <code>plot_3rd_axis</code> and <code>clip_along_third-axis</code> that are characters strings reading YES or NO. |

TIC_TYPE

TIC_TYPE sets the relative length of the tic marks.

| Syntax |
|--------------------------------------------------------------------------------------------------------------------------------------|
| <code>TIC_TYPE #</code> |
| <code>#</code> is a real number. Default value is 1. Negative number gives tics on the inside of the diagram frame. 0 gives no tics. |

TITLE

TITLE sets the title text string to be printed above the diagram.

| Syntax |
|--------------------------------------------------------------------------------------|
| <code>TITLE text</code> |
| <code>text</code> is an arbitrary text string that may contain text-formatting codes |

XLENGTH

XLENGTH sets the X-axis length to approximately # centimeters.

| | |
|--------|-----------------------------------------------------------------------------|
| Syntax | XLENGTH # |
| | # is a positive real number (the approximate X-axis length in centimeters). |

XSCALE

XSCALE sets the scaling in word coordinates of the X-axis.

| | |
|--------|-------------------------------|
| Syntax | XSCALE min max |
| | min and max are real numbers. |

XTEXT

XTEXT sets the X-axis text.

| | |
|--------|--------------------------------------------------------------------------|
| Syntax | XTEXT text |
| | text is an arbitrary text string that may contain text-formatting codes. |

XTYPE

XTYPE sets the X-axis type as linear (default), logarithmic or inverse.

| | |
|--------|-----------------------------------------------------|
| Syntax | XTYPE type |
| | type is a character string reading LIN, LOG or INV. |

YLENGTH

YLENGTH sets the Y-axis length to approximately # centimeters.

| | |
|--------|-----------------------------------------------------------------------------|
| Syntax | Y LENGTH # |
| | # is a positive real number (the approximate Y-axis length in centimeters). |

YSCALE

YSCALE sets the scaling in word coordinates of the Y-axis.

| | |
|--------|---------------------------------------------------------|
| Syntax | <code>YSCALE min max</code> |
| | <code>min</code> and <code>max</code> are real numbers. |

YTEXT

YTEXT sets the Y-axis text.

| | |
|--------|---------------------------------------------------------------------------------------|
| Syntax | <code>Y TEXT text</code> |
| | <code>text</code> is an arbitrary text string that may contain text-formatting codes. |

YTYPE

YTYPE sets the Y-axis type as linear (default), logarithmic or inverse.

| | |
|--------|------------------------------------------------------------------|
| Syntax | <code>Y TYPE type</code> |
| | <code>type</code> is a character string reading LIN, LOG or INV. |

DATASET Commands

In this section:

| | |
|------------------|----|
| ATTRIBUTE | 21 |
| BLOCK | 21 |
| BLOCKEND | 22 |
| CHARSIZE | 22 |
| CLIP | 22 |
| COLOR | 23 |
| DATASET | 24 |
| DATAPOINT | 24 |
| DRAWLINE | 24 |
| FONT | 25 |
| FUNCTION | 25 |
| GLOBALSIZE | 26 |
| INCLUDE | 26 |
| LINETYPE | 26 |
| PAINT | 27 |
| PCFUNCTION | 27 |
| SYMBOLSIZE | 28 |
| STRING | 28 |
| TEXT | 29 |

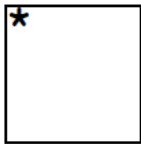
ATTRIBUTE

ATTRIBUTE specifies where the current XY position is in the character or symbol plotbox.

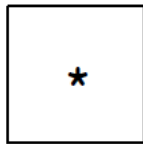


["Example 2 – Draw Polygons and Symbols" on page 32](#), ["Example 3 – Using Strings and Various Line Types" on page 34](#), and ["Example 5 – Use Included Files for Predefined Symbols" on page 38](#)

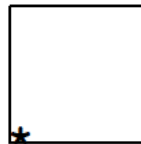
| Syntax | ATTRIBUTE |
|---------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Prompts | <code>attribute</code> |
| | <code>attribute</code> may be TOP, CENTER or BOTTOM. ATTRIBUTE CENTER is default for symbols; ATTRIBUTE BOTTOM is default for characters. |



TOP



CENTER



BOTTOM

BLOCK

BLOCK defines how the following numeric data block shall be interpreted. The definitions of X and Y coordinates may also be expressed as a function of the column values, making it possible to perform transformations.

| Syntax | <code>BLOCK X&=C#; ...; Y&=C#; ...; GOC=C#,@@@...</code> |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <code>&'</code> are optional unsigned integers that make it possible to plot several (maximum 9) X- or Y- axis columns. <code>#'</code> are unsigned integers identifying the column numbers. The column number <code>#</code> in " <code>GOC=C#</code> " is the location of any possible GOC codes in the current data BLOCK; <code>@@@</code> stands for the default Graphical Operation Code (GOC) for the current BLOCK. The GOC code inside the current table is only necessary if the current default GOC is not applicable. |

GOC CHARACTERS

The GOC is a combination of the following characters:

| Character | Meaning |
|---------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| <code>w</code> , <code>v</code> or <code>N</code> | To use word (<code>w</code>), virtual (<code>v</code>) or normalized (<code>N</code>) coordinates. <code>w</code> is the default. |
| <code>A</code> or <code>R</code> | XY are absolute (<code>A</code>) or relative (<code>R</code>) values. <code>A</code> is the default. |

| Character | Meaning |
|-----------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| M or D | To perform a move (M) or draw (D) operation to XY. M is the default. |
| B | To apply “soft” splines on a line drawn between the coordinate pairs (used only on BLOCK data). |
| S | To plot default symbol at XY. |
| S# | To change default symbol to No # symbol and plot it at XY. |
| `TEXT | To plot TEXT at XY. It must be the last operation in a GOC code. The TEXT following the ' command is interpreted and expanded by the DIGLIB software, if it includes any ^ operator or STRING names using the ~ descriptor. |

BLOCKEND

| Syntax | BLOCKEND |
|--------|----------------------------------------------------------------------------------------------------------------|
| | BLOCKEND terminates the local definition of the graphical operation code defined by the earlier BLOCK command. |

CHARSIZE

CHARSIZE redefines the default size of the characters in the plot. The character size has an initial default value, which may vary with the current font setting and the output device (the plot format).



["Examples of DATAPLOT Files and Outputs" on page 30](#)

| Syntax | CHARSIZE \$\$ |
|--------|--------------------------------|
| | \$\$ must be an unsigned real. |

CLIP

CLIP turns clipping on or off. If it is OFF, it allows output outside the ordinary plot area defined by normalized coordinates zero and one.



["Example 2 – Draw Polygons and Symbols" on page 32](#) and ["Example 9 - DIGLIB Fonts and Lines" on page 59](#)

| Syntax | CLIP CLP |
|--------|----------------------------------------------|
| | clp is a character string reading ON or OFF. |

COLOR

COLOR redefines the current color setting. There are 22 legal color codes (from 0 to 21).



["Example 7 – Color Codes" on page 46](#)

Syntax

COLOR `code`

`code` is an unsigned integer number (from 0 to 21) identifying the color, or a character string specifying the color.

DIGLIB COLOR CODES

| Code | Color | Equivalent Character |
|------|------------|----------------------|
| 0 | Background | Invisible |
| 1 | Black | Normal |
| 2 | Red | Very_Thick |
| 3 | Green | Thin |
| 4 | Blue | Thick |
| 5 | Yellow | Very_Thin |
| 6 | Magenta | Dashed |
| 7 | Cyan | Dotted |
| 8 | Purple | |
| 9 | Gold | |
| 10 | Turquoise | |
| 11 | Pink | |
| 12 | Gray | |
| 13 | Orange-red | |
| 14 | Maroon | |
| 15 | Plum | |
| 16 | Sea green | |
| 17 | Olive | |

| Code | Color | Equivalent Character |
|---------------|-------------------------------------------------------------|----------------------|
| 18 | Sienna | |
| 19 | Orange | |
| 20 | Coral | |
| 21 | UserDef | |
| 22 and higher | Any digit larger than 21 has the color effect as 1 (black). | |

DATASET

DATASET indicates the beginning of a number of consequent lines comprising a set of user-defined data. The DATASET lines are displayed on the terminal along with the `optional text` when using the `-1` option in the POST-processor as prompted for the DATASET number in the ["APPEND EXPERIMENTAL DATA" on page 353](#) or ["QUICK EXPERIMENTAL PLOT" on page 362](#) command.

| Syntax | DATASET # optional text |
|--------|--------------------------------------------------------|
| | # is an unsigned integer identifying this set of data. |

DATAPoint

DATAPoint is not a DATASET command, but the basic DATAPLOT command (see synopsis below) performs an action at the current point determined by the specified X/Y- coordinates. A DATASET may contain various data points, in addition to one or more data ["BLOCK" on page 21s](#). Such data points are separated and independent on each other.

| Syntax | X Y GOC |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | X and Y are unsigned real numbers identifying the X/Y-coordinates for the current data point. GOC stands for Graphical Operation Code (GOC) for the current point. Legal GOC characters. |
| | EXAMPLE |
| | 0.7 0.95 N'Example 6 |
| | 0.5 0.08 MNA'E^FS18^SQ(^SK^FS10A+5#8*C#^FS10 -!a^FS18)^FS11+B^Dla#b#s |

DRAWLINE

DRAWLINE draws a line starting at (x1,y1) to (xn,yn) through (x2,y2) → (x(n-1), y(n-1)).



["Example 1 – Draw Lines and Symbols" on page 31](#) and ["Example 2 – Draw Polygons and Symbols" on page 32](#)

| Syntax | <code>DRAWLINE x1,y1 x2,y2 xn,yn</code> | | | | | | | | | | | | |
|------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------|-----------------|----------------|-----------------|-----------------|----------------|------------------|------------------|----------------|-----------------|-----------------|----------------|
| | <p><code>x</code> and <code>y</code> may be reals or integers of any value. This is the same as connecting all points in a table:</p> <table><tr><td><code>x1</code></td><td><code>y1</code></td><td><code>M</code></td></tr><tr><td><code>x2</code></td><td><code>y2</code></td><td><code>D</code></td></tr><tr><td><code>...</code></td><td><code>...</code></td><td><code>D</code></td></tr><tr><td><code>xn</code></td><td><code>yn</code></td><td><code>D</code></td></tr></table> | <code>x1</code> | <code>y1</code> | <code>M</code> | <code>x2</code> | <code>y2</code> | <code>D</code> | <code>...</code> | <code>...</code> | <code>D</code> | <code>xn</code> | <code>yn</code> | <code>D</code> |
| <code>x1</code> | <code>y1</code> | <code>M</code> | | | | | | | | | | | |
| <code>x2</code> | <code>y2</code> | <code>D</code> | | | | | | | | | | | |
| <code>...</code> | <code>...</code> | <code>D</code> | | | | | | | | | | | |
| <code>xn</code> | <code>yn</code> | <code>D</code> | | | | | | | | | | | |

FONT

FONT redefines the default font setting in the POST-processor.



["Example 9 - DIGLIB Fonts and Lines" on page 59](#)

| Syntax | FONT # |
|--------|---------------------------|
| | # is an unsigned integer. |

Font Numbers

| Number | Font |
|--------|--------------------------|
| 1 | Bold |
| 2 | Normal |
| 3 | Italic |
| 5 | Bold and Italic |
| 10 | Monotype Normal |
| 11 | Monotype Italic |
| 12 | Monotype Bold |
| 13 | Monotype Bold and Italic |
| 14 | Narrow Normal |
| 15 | Narrow Italic |

FUNCTION

FUNCTION defines and plots a user-defined function.



["Example 4 – Draw Curves Defined by Functions" on page 36](#)

| | |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | <pre>FUNCTION Y=f(X); start end number_of_XY_pairs; GOC; FUNCTION X=f(Y); start end number_of_XY_pairs; GOC;</pre> |
| | <p>$f(X)$ or $f(Y)$ are legal mathematical functions of X or Y, understandable by a FORTRAN program. <code>start</code> and <code>end</code> are unsigned real numbers, and <code>number_of_XY_pairs</code> an unsigned integer. <code>GOC</code> is a legal graphical operation code as defined with "BLOCK" on page 21.</p> |

GLOBALSIZE

GLOBALSIZE redefines the default global size of the plot. The global size has an initial default value.

| | |
|--------|--------------------------------|
| Syntax | GLOBALSIZE \$\$ |
| | \$\$ must be an unsigned real. |

INCLUDE

INCLUDE adds a file into the current input stream.



["Example 5 – Use Included Files for Predefined Symbols" on page 38](#).

| | |
|--------|--------------------------------------------------------------------------------|
| Syntax | INCLUDE filename |
| | filename is a legal filename (with its correct path) for the operation system. |

LINETYPE

LINETYPE redefines the current linetype in the plot.



["Example 3 – Using Strings and Various Line Types" on page 34](#), ["Example 8 - DIGLIB Symbols" on page 51](#) and ["Example 9 - DIGLIB Fonts and Lines" on page 59](#)

| | |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Syntax | LINETYPE # |
| | <p># must be an unsigned integer. Legal linetypes are (for both normal graphical outputs and for PostScript formats):</p> <ul style="list-style-type: none"> • Solid (default) • Long dashed • Short dashed • Dotted |

Line Types

| Number | Type |
|--------|---------------|
| 1 | Straight line |
| 2 | Dashed line |
| 3 | Dotted line |
| 4 | Dash-Dot line |

PAINT

PAINT paints the area enclosed by the current path in the current pattern. The current path starts at the last MOVETO given and includes all subsequent DRAWs. This command only works for the PostScript format (as graphical files or on printed hardcopy).

► ["PCFUNCTION" below](#)

| Syntax | PAINT <code> <video> <mode> |
|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p><> denotes optional parameters. To set a new current pattern, supply any or all of the optional parameters.</p> <ul style="list-style-type: none">• <code> is a single letter 0-9, A-Z or a-t (if <code>=t, also supply a space and a number in the range 0.00-1.00). The default is 0.• <video> is a string reading NORMAL (the default) or INVERSE.• <mode> is a string reading TRANSPARENT (the default) or OPAQUE. |

PCFUNCTION

PCFUNCTION appends a user-defined function to the current path. It is used with ["PAINT" above](#).

| Syntax | PCFUNCTION Y=f(X); start end number_of_XY_pairs; GOC; PCFUNCTION X=f(Y); start end number_of_XY_pairs; GOC; |
|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| | <p>f(X) or f(Y) are legal mathematical functions of X or Y, understandable by a FORTRAN program. start and end are unsigned real numbers, and number_of_XY_pairs an unsigned integer. GOC is a legal graphical operation code as defined with "BLOCK" on page 21.</p> |

SYMBOLSIZE

SYMBOLSIZE redefines the current symbol size setting. The symbol size has an initial default value.



["Example 3 – Using Strings and Various Line Types" on page 34](#), ["Example 7 – Color Codes" on page 46](#) and ["Example 8 - DIGLIB Symbols" on page 51](#)

| Syntax |
|---------------------------------------------|
| <code>SYMBOLSIZE \$\$</code> |
| <code>\$\$</code> must be an unsigned real. |

STRING

STRING defines a string containing a text and operation codes (e.g., to change the default font settings).



["Example 3 – Using Strings and Various Line Types" on page 34](#) and ["Example 5 – Use Included Files for Predefined Symbols" on page 38](#)

| Syntax |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>STRING name text_with_each_character_in_^S#^G^F#^U#^D#^R#^L#^N</code> |
| <p><code>name</code> is a valid alphanumeric name (variable) to represent the text including all text formatting codes. It is highly recommended that all the characters in the name are in CAPITAL CASE (e.g. ACA2SO4); otherwise, the defined STRING can be incorrectly plotted.</p> <p><code>text_with_each_character_in_^S#^G^F#^U#^D#^R#^L#^N</code></p> <p>means the text is coded with each of its characters (and/or numeric numbers) that are formatted with various operators (<code>^S#</code>, <code>^G</code>, <code>^F#</code>, <code>^U#</code>, <code>^D#</code>, <code>^R#</code>, <code>^L#</code> and/or <code>^N</code>). <code>#</code>' are unsigned integers. <code>^</code> is the caret character and does not mean a control character. Between an <code>#</code> (in an operator) and a numeric number (as a part of the text), there must always be a comma sign (,) or the number is not plotted in the text, because the <code>#</code> with the number is interpreted as another incorrect <code>#</code>. In some of the commands, <code>#=0</code> resets the option to previous (or default) value.</p> |

STRING OPERATION CODES IN THE DIGLIB SOFTWARE

For the PostScript hardcopy fonts, these operation codes are not valid; see ["LaTeX Formatting Codes" on page 14](#):

| Operator | Operation |
|----------|--------------------------------|
| ^S# | Set character size to size # |
| ^G | Set font to Greek |
| ^F# | Set font to font number # |
| ^U# | Move up # units |
| ^D# | Move down # units |
| ^R# | Move right # units |
| ^L# | Move left # units |
| ^N | Do not move, remain at current |

EXAMPLES

```
STRING Alpha1 ^Ga^F0^D0^S8,1^S0^U0
```

is set to α_1

```
STRING M23C6 M^D0^S8,23^S0^U0C^D0^S8,6^S0^U0
```

is set to $M_{23}C_6$

```
STRING ACA2CO3 ^Ga^F0^D0^S8Ca^D0^S4,2^S0^U0^S8CO^D0^S4,3^S0^U0
```

is set to Ca_2CO_3

TEXT

TEXT outputs, at the current position, the text following the keyword TEXT or the text in the string `string_name` that is defined with ["STRING" on the previous page](#).

| Syntax | TEXT text or ~string_name |
|--------|---------------------------------------------------------------------------------------------|
| | It is possible to mix ^ operators and previously defined string names using the ~ operator. |

Examples of DATAPLOT Files and Outputs

Once your Thermo-Calc software is installed you can open the Examples and PDF documentation (Manuals) from the main menu:

- To open the Manuals folder select **Help → Manuals Folder**. Note for Linux openSUSE users: This link is not functional. To access the folder, navigate to the default location based on your installation type
- To open the Examples based on whether you are in Console Mode or Graphical Mode, select **File → Examples Files** or **Help → Examples Files**.

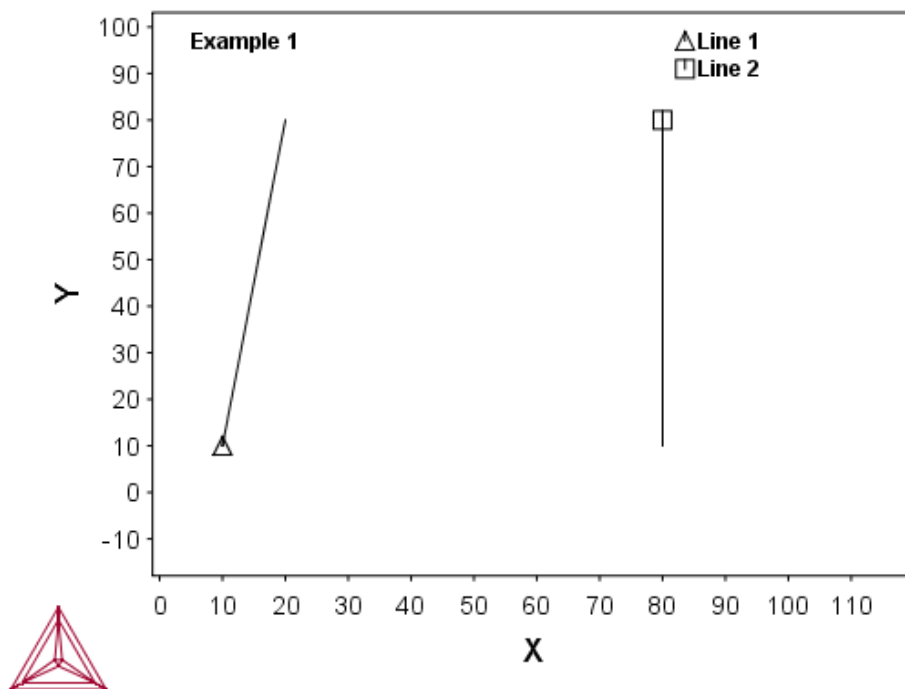
In this section:

| | |
|-------------------------------------------------------------|----|
| Example 1 – Draw Lines and Symbols | 31 |
| Example 2 – Draw Polygons and Symbols | 32 |
| Example 3 – Using Strings and Various Line Types | 34 |
| Example 4 – Draw Curves Defined by Functions | 36 |
| Example 5 – Use Included Files for Predefined Symbols | 38 |
| Example 6 – Triangular Diagrams for Ternary Systems | 40 |
| Example 7 – Color Codes | 46 |
| Example 8 - DIGLIB Symbols | 51 |
| Example 9 - DIGLIB Fonts and Lines | 59 |

Example 1 – Draw Lines and Symbols

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 1 - Draw Lines and Symbols.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help** → **Manuals Folder**.

Output Example



Macro Text

```
DATAPLOT Example 1
PROLOG 1 EXAMPLE 1 0<X<100, 0<Y<100
XSCALE 0.00000 100
YSCALE 0.00000 100
XTYPE LINEAR
YTYPE LINEAR
XLENGTH 11.5000
YLENGTH 11.5000
TITLE EXAMPLE 1
XTEXT X
```

```

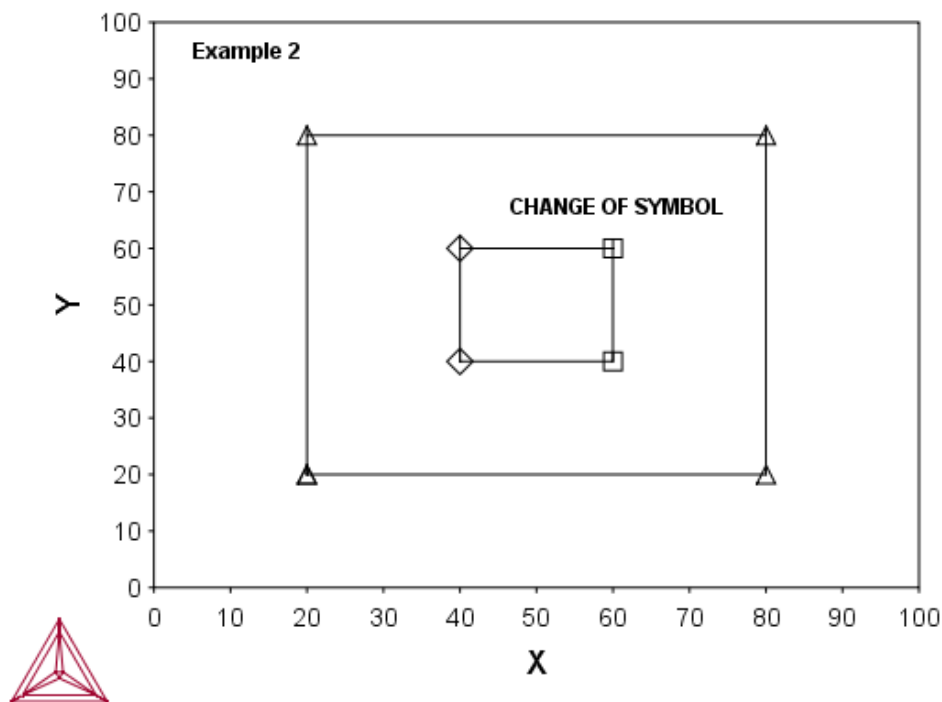
YTEXT Y
DATASET 1 Two lines started with two symbols
ATTRIBUTE CENTER
0.05 0.95 N'Example 1
0.7 0.95 NS'Line 1
0.7 0.90 NS2'Line 2
10 10 S1
20 80 D
80 80 S2
80 10 D
50 60

```

Example 2 – Draw Polygons and Symbols

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 2 - Draw Polygons and Symbols.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example



Macro Text

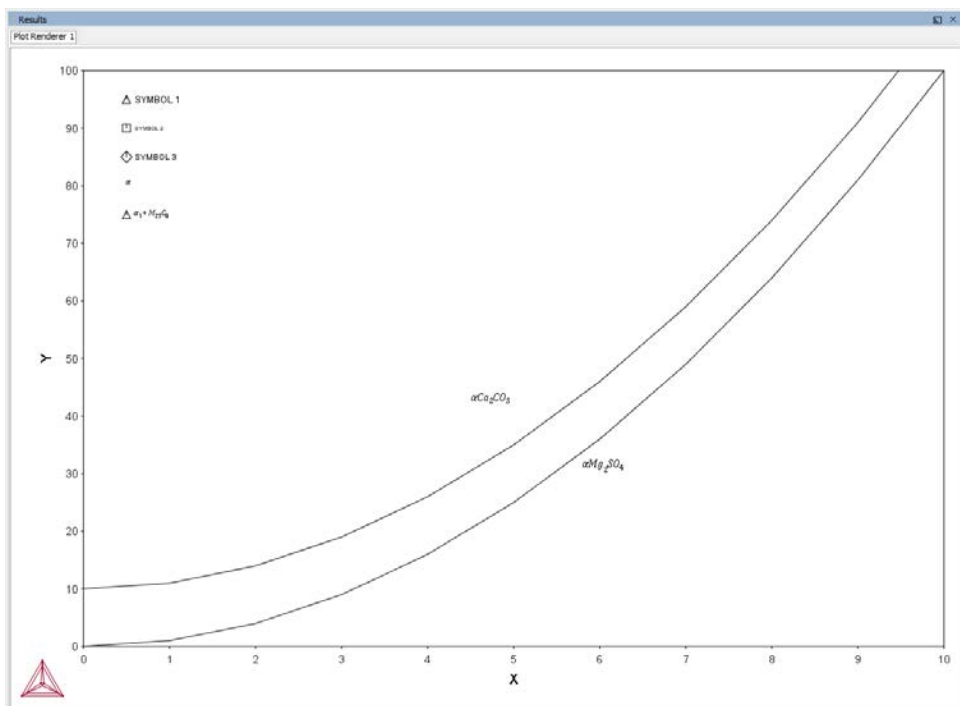
```
$DATAPLOT Example 2
PROLOG 2 EXAMPLE 2 0<X<100, 0<Y<100
XSCALE 0.00000 100
YSCALE 0.00000 100
XTYPE LINEAR
YTYPE LINEAR
XLENGTH 11.5000
YLENGTH 11.5000
TITLE EXAMPLE 2
XTEXT X
YTEXT Y
DATASET 2 Two ploygons with three types of symbols
ATTRIBUTE CENTER
CLIP OFF
0.05 0.95 N'Example 2
1.1 0.95 NS1'SYMBOL 1
1.1 0.90 NS2'SYMBOL 2
1.1 0.85 NS3'SYMBOL 3
BLOCK X=C1; Y=C2; GOC=C3,DSWA
40 40 M
40 60
60 60 S2'CHANGE OF SYMBOL
60 40
40 40 S0
BLOCKEND
BLOCK X=C1*100; Y=C2*100; GOC=C3,DSWA
0.2 0.2 MS1
0.2 0.8
0.8 0.8
0.8 0.2
0.2 0.2
BLOCKEND
$Draw an additional polygon:
DRAWLINE 20,10 30,15 40,30 50,80
```

DRAWLINE 50,80 60,60 90,30

Example 3 – Using Strings and Various Line Types

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file DATAPLOT 3 – Using String and Line Types.EXP available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example



Macro Text

```
$DATAPLOT Example 3
PROLOG 3 EXAMPLE 3 0<X<10, 0<Y<100
XSCALE 0.00000 10
YSCALE 0.00000 100
XTYPE LINEAR
YTYPE LINEAR
XLENGTH 11.5000
YLENGTH 11.5000
TITLE EXAMPLE 3
XTEXT X
```

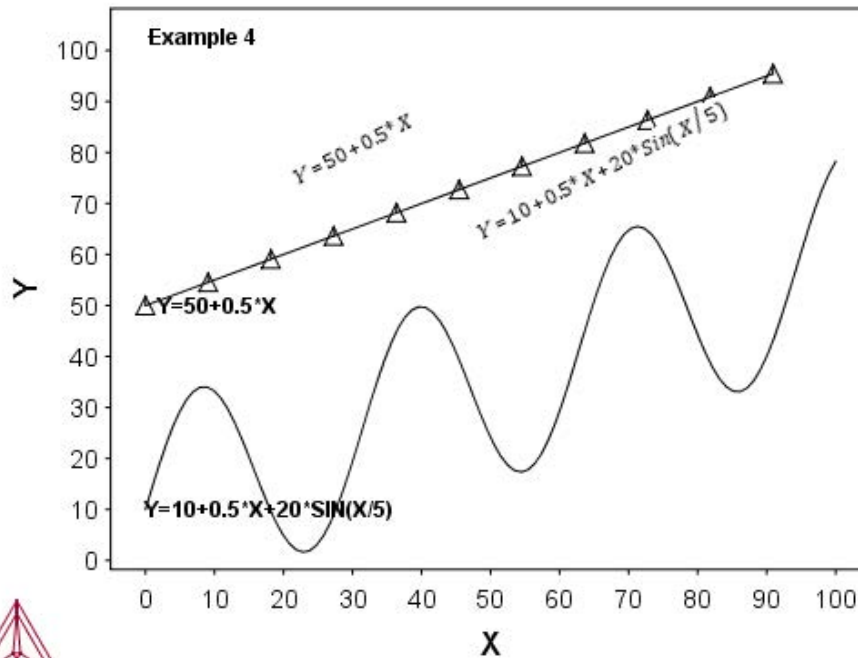
```
YTEXT Y
DATASET 3 Draw curves; plot formatted texts and symbols
$Define some strings:
STRING BCC \latex \alpha
STRING BCC1 \latex \alpha_1 + M_{23C_8}
STRING M23C6 M_{23C_6}
STRING ACA2CO3 \latex \alpha Ca_2CO_3
STRING AMG2SO4 \latex \alpha Mg_2SO_4
ATTRIBUTE CENTER
CLIP OFF
FONT 2
0.05 0.95 NS1'SYMBOL 1
CHARSIZE 0.2
0.05 0.90 NS2' SYMBOL 2
CHARSIZE 0.3
0.05 0.85 NS3'SYMBOL 3
0.05 0.80 N' ~BCC
0.05 0.75 NS1'~BCC1
SYMBOLSIZE 0.4
CHARSIZE 0.4
0.45 0.42 N'~ACA2CO3
0.58 0.30 N'~AMG2SO4
CLIP ON
LINETYPE 1
BLOCK X=C1; Y=C1*C1; GOC=C2, DWA
0 M
1
2
3
4
5
6
7
8
9
```

```
10
BLOCKEND
LINETYPE 2
BLOCK X=C1; Y=C1*C1+10; GOC=C2, DWA
0 M
1
2
3
4
5
6
7
8
9
10
BLOCKEND
```

Example 4 – Draw Curves Defined by Functions

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 4 - Curves and Functions.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example



Macro Text

```
$DATAPLOT Example 4
PROLOG 4 EXAMPLE 4 0<X<100, 0<Y<100
XSCALE 0.00000 100
YSCALE 0.00000 100
XTYPE LINEAR
YTYPE LINEAR
XLENGTH 11.5000
YLENGTH 11.5000
TITLE EXAMPLE 4
XTEXT X
YTEXT Y
DATASET 4 Plot two functions as lines:
ATTRIBUTE CENTER
0.05 0.95 N'Example 4
$ Draw two lines defined by FUNCTIONS:
FUNCTION Y=10+0.5*X+20*Sin(X/5); 0 100 100; DWA;
```

```
FUNCTION Y=50+0.5*X; 0 100 10; DS1WA;  
$ Write functions beside the lines:  
$ Note the real rotation angle (27 degree) can be seen  
$ only on the PostScript hardcopy  
0.25 0.68 N'^R027Y=50+0.5*X  
0.25 0.45 N'^R027Y=10+0.5*X+20*Sin(X/5)
```

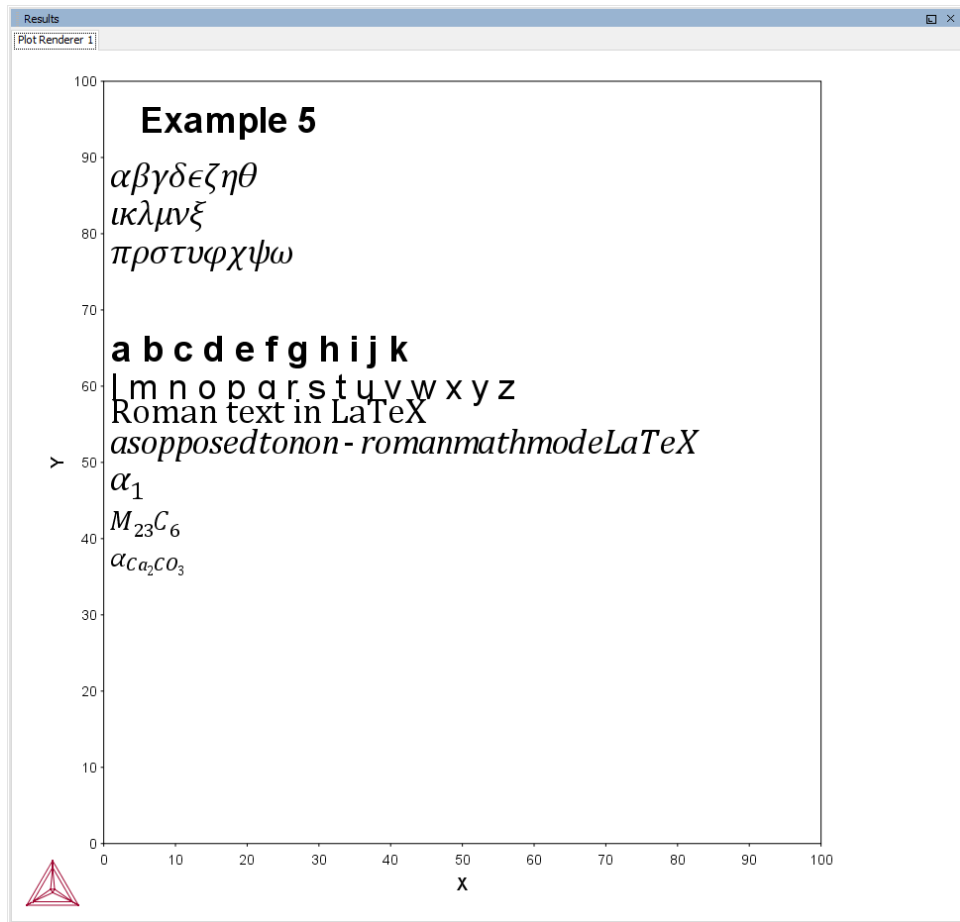
Example 5 – Use Included Files for Predefined Symbols

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 5 - Predefined Symbols.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example



In the plot result, the hard-to-read LaTeX line is intended to highlight how to type readable text using LaTeX.



Macro Text

```
$DATAPLOT Example 5 Symbols
PROLOG 5 EXAMPLE 5 0<X<100, 0<Y<100
XSCALE 0.00000 100
YSCALE 0.00000 100
XTYPE LINEAR
YTYPE LINEAR
XLENGTH 11.5000
YLENGTH 11.5000
TITLE EXAMPLE 5
XTEXT X
YTEXT Y
DATASET 5 Write equations and strings with different properties
STRING TEST1A \latex \alpha \beta \gamma \delta \epsilon \zeta \eta \theta
STRING TEST1B \latex \iota \kappa \lambda \mu \nu \xi \omicron
```

```

STRING TEST1C \latex \pi \rho \sigma \tau \upsilon \phi \chi \psi \omega
STRING TEST2A a b c d e f g h i j k
STRING TEST2B l m n o p q r s t u v w x y z
STRING BCC1 \latex \alpha_1
STRING ACA2CO3 \latex \alpha_{Ca_2CO_3}
ATTRIBUTE CENTER
CHARSIZE 1
0.05 0.95 N'Example 5
CLIP OFF
0.01 0.85 N'~TEST1A
0.01 0.80 N'~TEST1B
0.01 0.75 N'~TEST1C
FONT 1
0.01 0.65 N'~TEST2A
FONT 2
0.01 0.60 N'~TEST2B
0.01 0.55 N'\latex \textrm{Roman text in LaTeX}
0.01 0.50 N'\latex as opposed to non-roman math mode LaTeX
0.01 0.45 N'~BCC1
CHARSIZE 0.8
0.01 0.40 N'\latex M_{23}C_6
0.01 0.35 N'~ACA2CO3

```

Example 6 – Triangular Diagrams for Ternary Systems

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 6 - Ternary Plots.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example



In the DATAPLOT language, this type of diagram is only available for Console Mode.

DATASET 6 Plot a ternary phase diagram

CLIP OFF

0.80 0.90 N'Example 6

0.86 0.31 N'B2C

0.52 0.97 N'Diamond

CHARSIZE 0.25

1.4E+01 1.10E+01 MVA'1:*B2C Liquid

1.4E+01 1.05E+01 MVA'2:*Diamond Liquid

0.10 0.10 N'Liquid

0.48 0.45 N'Diamond+

0.48 0.40 N' B2C+Liquid

5.80E-01 5.40E-02 MWA' 1

1.90E-01 2.40E-01 MWA' 1

0.65E-01 2.50E-01 MWA' 2

CHARSIZE 0.45

-0.10 -0.05 N'A

1.06 -0.05 N'B

0.48 1.05 N'C

CHARSIZE 0.35

\$\$ Calculated A-B-C Phase Equilibrium Data:

\$ PHASE REGION FOR:

\$F0 LIQUID

\$E DIAMOND_A4

\$F0 B2C

\$ INVARIANT EQUILIBRIUM

COLOR 2

BLOCK X=C1; Y=C2; GOC=C3,WAD;

2.4555855989E-01 3.5568857193E-01 M
0.0000000000E+00 9.9999523163E-01
2.4555855989E-01 3.5568857193E-01 M
6.6666668653E-01 3.3333334327E-01
0.0000000000E+00 9.9999523163E-01 M
6.6666668653E-01 3.3333334327E-01
COLOR 1
BLOCKEND
\$ PHASE REGION FOR:
\$E LIQUID
\$F0 B2C
BLOCK X=C1; Y=C2; GOC=C3,WAD;
\$ PLOTTED COLUMNS ARE : X(LIQUID,B) and X(LIQUID,C)
2.2030337155E-01 1.2340000272E-01 M
2.2632879019E-01 1.1058768630E-01
2.3371633887E-01 9.9345825613E-02
2.4253317714E-01 8.9345827699E-02
2.6429468393E-01 7.2744041681E-02
2.8429466486E-01 6.2814079225E-02
2.9617273808E-01 5.8319382370E-02
3.2811737061E-01 4.9470417202E-02
3.6353862286E-01 4.3130427599E-02
3.9895987511E-01 3.8979098201E-02
4.5209178329E-01 3.5266116261E-02
5.2293431759E-01 3.3152002841E-02
6.1148744822E-01 3.3077053726E-02
6.4690870047E-01 3.3490389585E-02

6.8232995272E-01 3.4017231315E-02
7.3546189070E-01 3.4814555198E-02
7.5317251682E-01 3.5033416003E-02
8.0630439520E-01 3.5373892635E-02
8.5943627357E-01 3.4983776510E-02
9.1256815195E-01 3.3575300127E-02
9.6747112274E-01 3.0857827514E-02
9.6922445297E-01 3.0749246478E-02
2.2030337155E-01 1.2340000272E-01 M
2.1294665337E-01 1.5308913589E-01
2.1171525121E-01 1.8851040304E-01
2.1532440186E-01 2.2393165529E-01
2.2180187702E-01 2.5935292244E-01
2.2992117703E-01 2.9477417469E-01
2.3888295889E-01 3.3019542694E-01
2.4555855989E-01 3.5568857193E-01
\$ PLOTTED COLUMNS ARE : X(B2C,B) and X(B2C,C)
6.6666668653E-01 3.3333334327E-01 M
6.6666668653E-01 3.3333334327E-01
\$ TIELINES
COLOR 3
6.6666668653E-01 3.3333334327E-01 M
8.7775242329E-01 3.4625384957E-02
6.6666668653E-01 3.3333334327E-01 M
7.9250496626E-01 3.5342670977E-02
6.6666668653E-01 3.3333334327E-01 M
2.4555824697E-01 3.5568737984E-01

6.6666668653E-01 3.3333334327E-01 M
2.3944084346E-01 9.2542596161E-02
6.6666668653E-01 3.3333334327E-01 M
2.3359020054E-01 3.0954307318E-01
6.6666668653E-01 3.3333334327E-01 M
2.2585247457E-01 2.7766343951E-01
6.6666668653E-01 3.3333334327E-01 M
2.1618695557E-01 1.3621240854E-01
2.2632879019E-01 1.1058768630E-01 M
6.6666668653E-01 3.3333334327E-01
COLOR 1
BLOCKEND
\$ PHASE REGION FOR:
\$F0 DIAMOND_A4
\$E B2C
BLOCK X=C1; Y=C2; GOC=C3,WAD;
\$ PLOTTED COLUMNS ARE : X(DIAMOND_A4,B) and X(DIAMOND_A4,C)
0.0000000000E+00 9.9999523163E-01 M
0.0000000000E+00 9.9999976158E-01
BLOCKEND
\$ PHASE REGION FOR:
\$E LIQUID
\$F0 DIAMOND_A4
BLOCK X=C1; Y=C2; GOC=C3,WAD;
\$ PLOTTED COLUMNS ARE : X(LIQUID,B) and X(LIQUID,C)
2.4555855989E-01 3.5568857193E-01 M
2.0263540745E-01 3.3483061194E-01

1.6243904829E-01 3.1375369430E-01

1.2243904918E-01 2.9153180122E-01

8.2439050078E-02 2.6854267716E-01

4.2439054698E-02 2.4548016489E-01

2.4390530307E-03 2.2313812375E-01

2.4999999937E-07 2.2181616724E-01

\$ TIELINES

COLOR 3

0.0000000000E+00 9.9999511242E-01 M

2.3529186845E-01 3.5085919499E-01

0.0000000000E+00 9.9999469519E-01 M

1.9826586545E-01 3.3260950446E-01

0.0000000000E+00 9.9999409914E-01 M

1.3240024447E-01 2.9716023803E-01

0.0000000000E+00 9.9999397993E-01 M

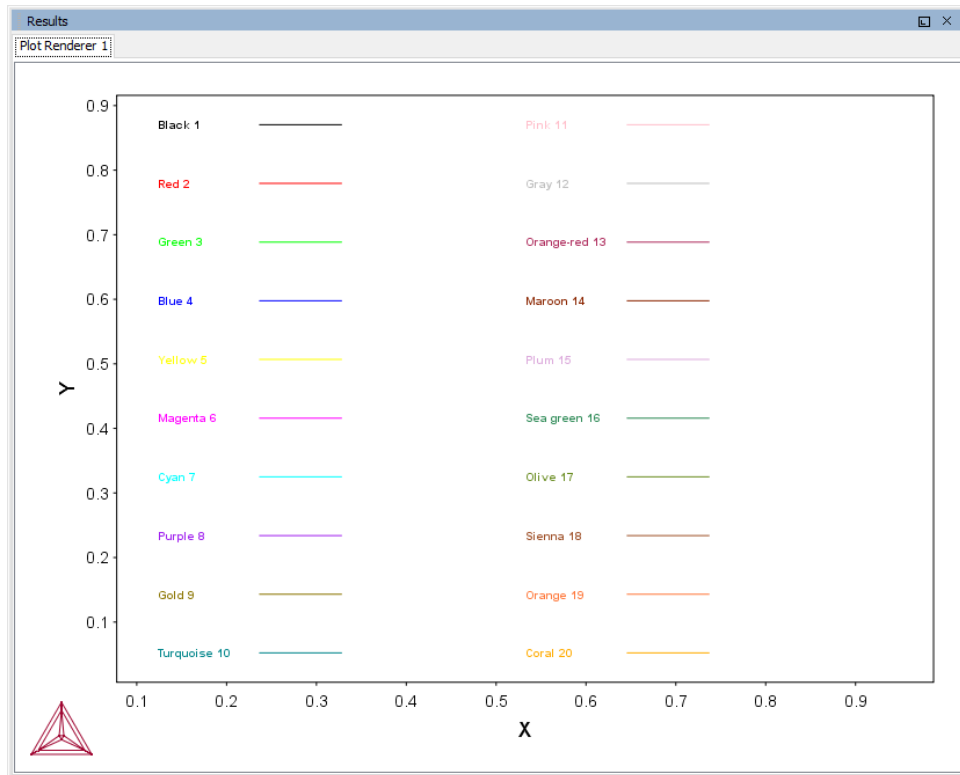
1.1439975351E-01 2.8695335984E-01

BLOCKEND

Example 7 – Color Codes

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 7 - Color Codes.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example



Macro Text

\$DATAPLOT Example 7 - DIGLIB Colors

PROLOG 1 DIGLIB Colors

XSCALE 0.0 1.0

YSCALE 0.0 1.0

XTYPE LINEAR

YTYPE LINEAR

XLENGTH 15.5000

YLENGTH 11.5000

TITLE DIGLIB Colors

XTEXT X

YTEXT Y

DATASET 1 DIGLIB Colors:

\$ DIGLIB Colors:

CHARSIZE 0.3

SYMBOLSIZE 0.5

```
COLOR 1
0.05 0.95 N' Black 1
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.95 M
0.275 0.95 D
BLOCKEND

COLOR 2
0.05 0.85 N' Red 2
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.85 M
0.275 0.85 D
BLOCKEND

COLOR 3
0.05 0.75 N' Green 3
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.75 M
0.275 0.75 D
BLOCKEND

COLOR 4
0.05 0.65 N' Blue 4
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.65 M
0.275 0.65 D
BLOCKEND

COLOR 5
0.05 0.55 N' Yellow 5
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.55 M
0.275 0.55 D
BLOCKEND

COLOR 6
0.05 0.45 N' Magenta 6
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.45 M
0.275 0.45 D
```

```
BLOCKEND
COLOR 7
0.05 0.35 N' Cyan 7
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.35 M
0.275 0.35 D
BLOCKEND
COLOR 8
0.05 0.25 N' Purple 8
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.25 M
0.275 0.25 D
BLOCKEND
COLOR 9
0.05 0.15 N' Gold 9
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.15 M
0.275 0.15 D
BLOCKEND
COLOR 10
0.05 0.05 N' Turquoise 10
BLOCK X=C1; Y=C2; GOC=C3,N
0.175 0.05 M
0.275 0.05 D
BLOCKEND
COLOR 11
0.5 0.95 N' Pink 11
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.95 M
0.725 0.95 D
BLOCKEND
COLOR 12
0.5 0.85 N' Gray 12
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.85 M
```

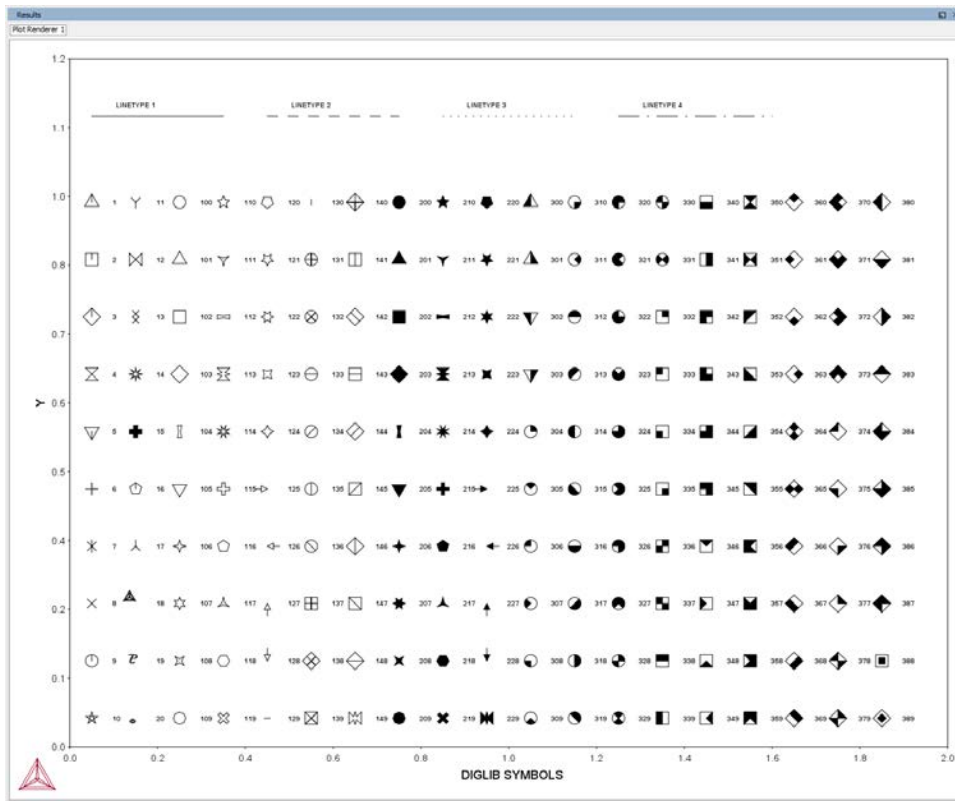
```
0.725 0.85 D
BLOCKEND
COLOR 13
0.5 0.75 N' Orange-red 13
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.75 M
0.725 0.75 D
BLOCKEND
COLOR 14
0.5 0.65 N' Maroon 14
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.65 M
0.725 0.65 D
BLOCKEND
COLOR 15
0.5 0.55 N' Plum 15
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.55 M
0.725 0.55 D
BLOCKEND
COLOR 16
0.5 0.45 N' Sea green 16
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.45 M
0.725 0.45 D
BLOCKEND
COLOR 17
0.5 0.35 N' Olive 17
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.35 M
0.725 0.35 D
BLOCKEND
COLOR 18
0.5 0.25 N' Sienna 18
BLOCK X=C1; Y=C2; GOC=C3,N
```

```
0.625 0.25 M
0.725 0.25 D
BLOCKEND
COLOR 19
0.5 0.15 N' Orange 19
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.15 M
0.725 0.15 D
BLOCKEND
COLOR 20
0.5 0.05 N' Coral 20
BLOCK X=C1; Y=C2; GOC=C3,N
0.625 0.05 M
0.725 0.05 D
BLOCKEND
```

Example 8 - DIGLIB Symbols

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 8 - DIGLIB Symbols.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example



A default symbol is the current symbol in the run of the software (it is usually the No 1 symbol if the POST-processor is switched on for the first time). S (i.e., # is not specified) means that the current symbol is plotted. S0 (i.e., #=0) means that no symbol is plotted.

Macro Text

```
$DATAPLOT DIGLIB Symbols 2
PROLOG 1 DIGLIB Symbols 2 0<X<2.0, 0<Y<1.2
XSCALE 0.0 2.0
YSCALE 0.0 1.2
XTYPE LINEAR
YTYPE LINEAR
XLENGTH 15.5000
YLENGTH 11.5000
TITLE DIGLIB Symbols
XTEXT DIGLIB SYMBOLS
DATASET 1 Various DIGLIB Symbols:
$ DIGLIB Symbols:
```

```
CHARSIZE 0.3
SYMBOLSIZE 0.5
0.05 0.95 WS1' 1
0.05 0.85 WS2' 2
0.05 0.75 WS3' 3
0.05 0.65 WS4' 4
0.05 0.55 WS5' 5
0.05 0.45 WS6' 6
0.05 0.35 WS7' 7
0.05 0.25 WS8' 8
0.05 0.15 WS9' 9
0.05 0.05 WS10' 10
0.15 0.95 WS11' 11
0.15 0.85 WS12' 12
0.15 0.75 WS13' 13
0.15 0.65 WS14' 14
0.15 0.55 WS15' 15
0.15 0.45 WS16' 16
0.15 0.35 WS17' 17
0.15 0.25 WS18' 18
0.15 0.15 WS19' 19
0.15 0.05 WS20' 20
0.25 0.95 WS100' 100
0.25 0.85 WS101' 101
0.25 0.75 WS102' 102
0.25 0.65 WS103' 103
0.25 0.55 WS104' 104
0.25 0.45 WS105' 105
0.25 0.35 WS106' 106
0.25 0.25 WS107' 107
0.25 0.15 WS108' 108
0.25 0.05 WS109' 109
0.35 0.95 WS110' 110
0.35 0.85 WS111' 111
0.35 0.75 WS112' 112
```

0.35 0.65 WS113' 113
0.35 0.55 WS114' 114
0.35 0.45 WS115' 115
0.35 0.35 WS116' 116
0.35 0.25 WS117' 117
0.35 0.15 WS118' 118
0.35 0.05 WS119' 119
0.45 0.95 WS120' 120
0.45 0.85 WS121' 121
0.45 0.75 WS122' 122
0.45 0.65 WS123' 123
0.45 0.55 WS124' 124
0.45 0.45 WS125' 125
0.45 0.35 WS126' 126
0.45 0.25 WS127' 127
0.45 0.15 WS128' 128
0.45 0.05 WS129' 129
0.55 0.95 WS130' 130
0.55 0.85 WS131' 131
0.55 0.75 WS132' 132
0.55 0.65 WS133' 133
0.55 0.55 WS134' 134
0.55 0.45 WS135' 135
0.55 0.35 WS136' 136
0.55 0.25 WS137' 137
0.55 0.15 WS138' 138
0.55 0.05 WS139' 139
0.65 0.95 WS140' 140
0.65 0.85 WS141' 141
0.65 0.75 WS142' 142
0.65 0.65 WS143' 143
0.65 0.55 WS144' 144
0.65 0.45 WS145' 145
0.65 0.35 WS146' 146
0.65 0.25 WS147' 147

| | | | |
|------|------|--------|-----|
| 0.65 | 0.15 | WS148' | 148 |
| 0.65 | 0.05 | WS149' | 149 |
| 0.75 | 0.95 | WS200' | 200 |
| 0.75 | 0.85 | WS201' | 201 |
| 0.75 | 0.75 | WS202' | 202 |
| 0.75 | 0.65 | WS203' | 203 |
| 0.75 | 0.55 | WS204' | 204 |
| 0.75 | 0.45 | WS205' | 205 |
| 0.75 | 0.35 | WS206' | 206 |
| 0.75 | 0.25 | WS207' | 207 |
| 0.75 | 0.15 | WS208' | 208 |
| 0.75 | 0.05 | WS209' | 209 |
| 0.85 | 0.95 | WS210' | 210 |
| 0.85 | 0.85 | WS211' | 211 |
| 0.85 | 0.75 | WS212' | 212 |
| 0.85 | 0.65 | WS213' | 213 |
| 0.85 | 0.55 | WS214' | 214 |
| 0.85 | 0.45 | WS215' | 215 |
| 0.85 | 0.35 | WS216' | 216 |
| 0.85 | 0.25 | WS217' | 217 |
| 0.85 | 0.15 | WS218' | 218 |
| 0.85 | 0.05 | WS219' | 219 |
| 0.95 | 0.95 | WS220' | 220 |
| 0.95 | 0.85 | WS221' | 221 |
| 0.95 | 0.75 | WS222' | 222 |
| 0.95 | 0.65 | WS223' | 223 |
| 0.95 | 0.55 | WS224' | 224 |
| 0.95 | 0.45 | WS225' | 225 |
| 0.95 | 0.35 | WS226' | 226 |
| 0.95 | 0.25 | WS227' | 227 |
| 0.95 | 0.15 | WS228' | 228 |
| 0.95 | 0.05 | WS229' | 229 |
| 1.05 | 0.95 | WS300' | 300 |
| 1.05 | 0.85 | WS301' | 301 |
| 1.05 | 0.75 | WS302' | 302 |

1.05 0.65 WS303' 303
1.05 0.55 WS304' 304
1.05 0.45 WS305' 305
1.05 0.35 WS306' 306
1.05 0.25 WS307' 307
1.05 0.15 WS308' 308
1.05 0.05 WS309' 309
1.15 0.95 WS310' 310
1.15 0.85 WS311' 311
1.15 0.75 WS312' 312
1.15 0.65 WS313' 313
1.15 0.55 WS314' 314
1.15 0.45 WS315' 315
1.15 0.35 WS316' 316
1.15 0.25 WS317' 317
1.15 0.15 WS318' 318
1.15 0.05 WS319' 319
1.25 0.95 WS320' 320
1.25 0.85 WS321' 321
1.25 0.75 WS322' 322
1.25 0.65 WS323' 323
1.25 0.55 WS324' 324
1.25 0.45 WS325' 325
1.25 0.35 WS326' 326
1.25 0.25 WS327' 327
1.25 0.15 WS328' 328
1.25 0.05 WS329' 329
1.35 0.95 WS330' 330
1.35 0.85 WS331' 331
1.35 0.75 WS332' 332
1.35 0.65 WS333' 333
1.35 0.55 WS334' 334
1.35 0.45 WS335' 335
1.35 0.35 WS336' 336
1.35 0.25 WS337' 337

| | | | |
|------|------|--------|-----|
| 1.35 | 0.15 | WS338' | 338 |
| 1.35 | 0.05 | WS339' | 339 |
| 1.45 | 0.95 | WS340' | 340 |
| 1.45 | 0.85 | WS341' | 341 |
| 1.45 | 0.75 | WS342' | 342 |
| 1.45 | 0.65 | WS343' | 343 |
| 1.45 | 0.55 | WS344' | 344 |
| 1.45 | 0.45 | WS345' | 345 |
| 1.45 | 0.35 | WS346' | 346 |
| 1.45 | 0.25 | WS347' | 347 |
| 1.45 | 0.15 | WS348' | 348 |
| 1.45 | 0.05 | WS349' | 349 |
| 1.55 | 0.95 | WS350' | 350 |
| 1.55 | 0.85 | WS351' | 351 |
| 1.55 | 0.75 | WS352' | 352 |
| 1.55 | 0.65 | WS353' | 353 |
| 1.55 | 0.55 | WS354' | 354 |
| 1.55 | 0.45 | WS355' | 355 |
| 1.55 | 0.35 | WS356' | 356 |
| 1.55 | 0.25 | WS357' | 357 |
| 1.55 | 0.15 | WS358' | 358 |
| 1.55 | 0.05 | WS359' | 359 |
| 1.65 | 0.95 | WS360' | 360 |
| 1.65 | 0.85 | WS361' | 361 |
| 1.65 | 0.75 | WS362' | 362 |
| 1.65 | 0.65 | WS363' | 363 |
| 1.65 | 0.55 | WS364' | 364 |
| 1.65 | 0.45 | WS365' | 365 |
| 1.65 | 0.35 | WS366' | 366 |
| 1.65 | 0.25 | WS367' | 367 |
| 1.65 | 0.15 | WS368' | 368 |
| 1.65 | 0.05 | WS369' | 369 |
| 1.75 | 0.95 | WS370' | 370 |
| 1.75 | 0.85 | WS371' | 371 |
| 1.75 | 0.75 | WS372' | 372 |

```
1.75 0.65 WS373' 373
1.75 0.55 WS374' 374
1.75 0.45 WS375' 375
1.75 0.35 WS376' 376
1.75 0.25 WS377' 377
1.75 0.15 WS378' 378
1.75 0.05 WS379' 379
1.85 0.95 WS380' 380
1.85 0.85 WS381' 381
1.85 0.75 WS382' 382
1.85 0.65 WS383' 383
1.85 0.55 WS384' 384
1.85 0.45 WS385' 385
1.85 0.35 WS386' 386
1.85 0.25 WS387' 387
1.85 0.15 WS388' 388
1.85 0.05 WS389' 389
$ DIGLIB Line Types:
LINETYPE 1
BLOCK X=C1; Y=C2; GOC=C3,DWA
0.05 1.10 M
0.35 1.10
BLOCKEND
LINETYPE 2
BLOCK X=C1; Y=C2; GOC=C3,DWA
0.45 1.10 M
0.75 1.10
BLOCKEND
LINETYPE 3
BLOCK X=C1; Y=C2; GOC=C3,DWA
0.85 1.10 M
1.15 1.10
BLOCKEND
LINETYPE 4
BLOCK X=C1; Y=C2; GOC=C3,DWA
```

```

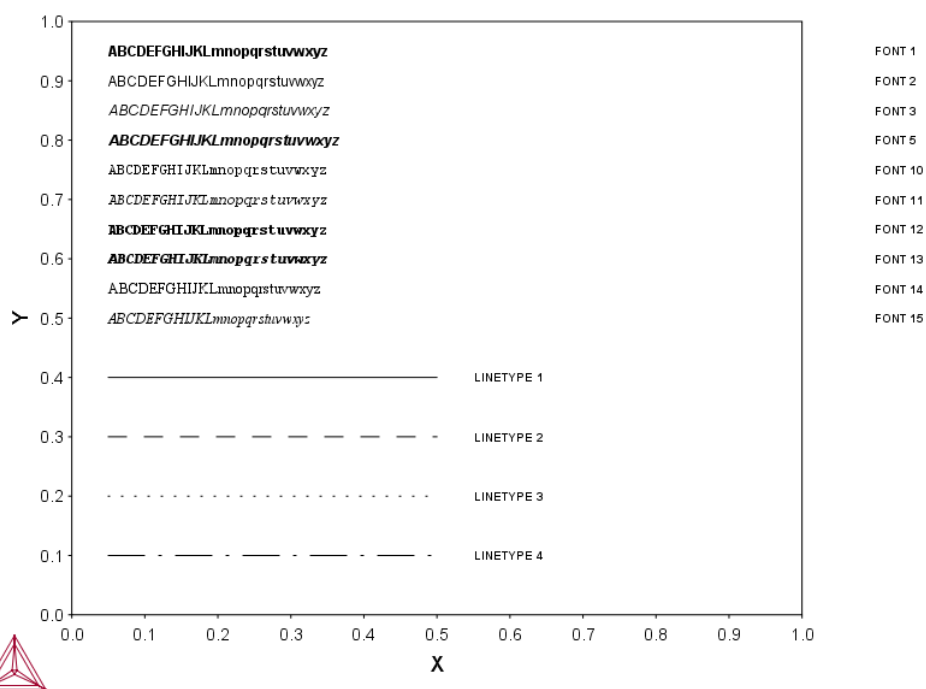
1.25 1.10 M
1.60 1.10
BLOCKEND
0.10 1.12 W' LINETYPE 1
0.50 1.12 W' LINETYPE 2
0.90 1.12 W' LINETYPE 3
1.30 1.12 W' LINETYPE 4

```

Example 9 - DIGLIB Fonts and Lines

The macro text below produces the example output. You can copy the text into your own EXP file, or use the example file `DATAPLOT 9 - DIGLIB Fonts.EXP` available with your installation. To open the folder: From the Thermo-Calc menu, select **Help → Manuals Folder**.

Output Example



Macro Text

```

$DATAPLOT Example 9 - DIGLIB Fonts
PROLOG 1 DIGLIB Fonts & Line Types 0<X<1, 0<Y<1
XSCALE 0.0 1.0
YSCALE 0.0 1.0

```

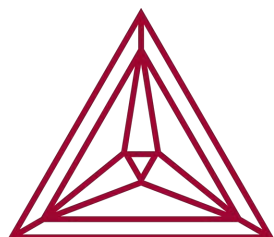
```
XTYPE LINEAR
YTYPE LINEAR
XLENGTH 11.5000
YLENGTH 11.5000
TITLE DIGLIB Fonts
XTEXT X
YTEXT Y
DATASET 1 Various DIGLIB Fonts and Line Types:
$ DIGLIB Fonts:
CHARSIZE .35
FONT 1
0.05 0.95 N'ABCDEFGHijklmnopqrstuvwxyz
FONT 2
0.05 0.90 N'ABCDEFGHijklmnopqrstuvwxyz
FONT 3
0.05 0.85 N'ABCDEFGHijklmnopqrstuvwxyz
FONT 5
0.05 0.80 N'ABCDEFGHijklmnopqrstuvwxyz
FONT 10
0.05 0.75 N'ABCDEFGHijklmnopqrstuvwxyz
FONT 11
0.05 0.70 N'ABCDEFGHijklmnopqrstuvwxyz
FONT 12
0.05 0.65 N'ABCDEFGHijklmnopqrstuvwxyz
FONT 13
0.05 0.60 N'ABCDEFGHijklmnopqrstuvwxyz
FONT 14
0.05 0.55 N'ABCDEFGHijklmnopqrstuvwxyz
FONT 15
0.05 0.50 N'ABCDEFGHijklmnopqrstuvwxyz
FONT 1
CLIP OFF
CHARSIZE .30
1.10 0.95 N'FONT 1
1.10 0.90 N'FONT 2
```

```
1.10 0.85 N'FONT 3
1.10 0.80 N'FONT 5
1.10 0.75 N'FONT 10
1.10 0.70 N'FONT 11
1.10 0.65 N'FONT 12
1.10 0.60 N'FONT 13
1.10 0.55 N'FONT 14
1.10 0.50 N'FONT 15
CLIP ON
$ DIGLIB Line Types:
LINETYPE 1
BLOCK X=C1; Y=C2; GOC=C3,DWA
0.05 0.40 M
0.50 0.40
BLOCKEND
$DRAWLINE 0.05,0.40 0.5,0.40
LINETYPE 2
BLOCK X=C1; Y=C2; GOC=C3,DWA
0.05 0.30 M
0.50 0.30
BLOCKEND
$DRAWLINE 0.05,0.30 0.5,0.30
LINETYPE 3
BLOCK X=C1; Y=C2; GOC=C3,DWA
0.05 0.20 M
0.50 0.20
BLOCKEND
$DRAWLINE 0.05,0.20 0.5,0.20
LINETYPE 4
BLOCK X=C1; Y=C2; GOC=C3,DWA
0.05 0.10 M
0.50 0.10
BLOCKEND
$DRAWLINE 0.05,0.10 0.5,0.10
0.55 0.40 N' LINETYPE 1
```

```
0.55 0.30 N' LINETYPE 2  
0.55 0.20 N' LINETYPE 3  
0.55 0.10 N' LINETYPE 4
```

Pourbaix Diagrams

Educational Material



Introduction to Pourbaix Diagrams

In this section:

| | |
|----------------------------------------------|---|
| About Pourbaix Diagrams in Thermo-Calc | 3 |
| Pourbaix Diagrams | 4 |
| Working with Pourbaix Diagrams | 6 |
| Key Concepts | 7 |
| Basic Settings and Definitions | 9 |

About Pourbaix Diagrams in Thermo-Calc

This guide is for Thermo-Calc software users who know the basics of thermodynamics and want to know more about ["Pourbaix Diagrams" on the next page](#).

You are introduced to the concept of a Pourbaix diagram and shown how to interpret such diagrams through a series of examples.

Materials corrosion occurs almost everywhere. It may lead to serious material damages, unexpected application failures, tremendous economic costs and environmental degradations. Consequently, scientists and engineers must often conduct expensive and time-consuming corrosion experiments as part of failure analyses, risk evaluations, quality improvements and application enhancements.

Under certain conditions, when a metal or alloy is exposed to an aqueous solution with a concentration of inorganic/organic mixture, corrosion phenomena occur at a corresponding degree. During corrosion, some metallic phases dissolve, the metal or alloy surface gets damaged and some secondary solid phases form at the solid-liquid interfaces (such as oxides, hydroxides, silicates, sulphides, sulphates, carbonates, nitrates, phosphates, borates, or halides). Such corrosive chemical or electrochemical reactions can be studied by means of the so-called Pourbaix diagrams if the reactions reach their equilibrium states (Pourbaix, 1973¹, 1974², 2003³, 2011⁴; Thompson et al. 2011⁵).

GES5 and GES6 Calculation Engine Version

As of Thermo-Calc version 2019b, the default calculation engine is set to GES6. For PARROT optimization and POURBAIX module users, you need to use GES5. When you try to enter these modules, you are instructed to switch to GES5 using the SET_GES_VERSION command.

► ["About the Gibbs Energy System \(GES\) Module" on page 36](#)

1. *Lectures on Electrochemical Corrosion*. Plenum Press, New York.

2. *Atlas of Electrochemical Equilibria in Aqueous Solutions*, 2nd Ed, Houston, Tex., National Association of Corrosion Engineers; Cramer and Covino.

3. *Corrosion: Fundamentals, Testing, and Protection*. ASM Handbook, Volume 13A; Verink.

4. "Simplified procedure for constructing Pourbaix diagrams", in: *Uhlig's Corrosion Handbook, 3rd Edition (Revie RW, Ed.)*, The Electrochemical Society and Jon Wiley & Sons, New Jersey

5. "Pourbaix diagrams for multielement systems", in: *Uhlig's Corrosion Handbook, 3rd Edition (Revie RW, Ed.)*, The Electrochemical Society and Jon Wiley & Sons, New Jersey



To globally set the default from GES6 back to GES5, go to the **Tools → Options** → **"General"** on [page 37](#) tab and click **Version 5** for the *Preferred Gibbs Energy System* setting. The **"SET GES VERSION"** on [page 118](#) Console Mode command is used to change GES versions for a single Thermo-Calc session.



Contact Thermo-Calc Software AB at info@thermocalc.com for more information about the changes or if you encounter any issues you think are related to the new version of the calculation engine.



GES6 is a re-write and new implementation of the Gibbs Energy System module of Thermo-Calc and it is the default engine. The previous version, GES5, is still available and will continue to work in the background of the program where necessary. The main purpose of GES6 is to support faster development of new features. However, not all GES5 functionality is implemented in GES6. In such cases (except for optimization, PARROT and the POURBAIX module), GES6 falls back silently and uses functionality from GES5 in the background.

Pourbaix Diagrams

Marcel Pourbaix applied thermodynamics to predict materials corrosion resistance. He determined the phase stability relations in terms of varied pH and Eh values for an interaction system of metal and pure water or dilute aqueous solution. He presented the stability regions of metal and secondary phases (such as metal-oxides/hydroxides) on a pH-Eh diagram, which is now known as a Pourbaix diagram.

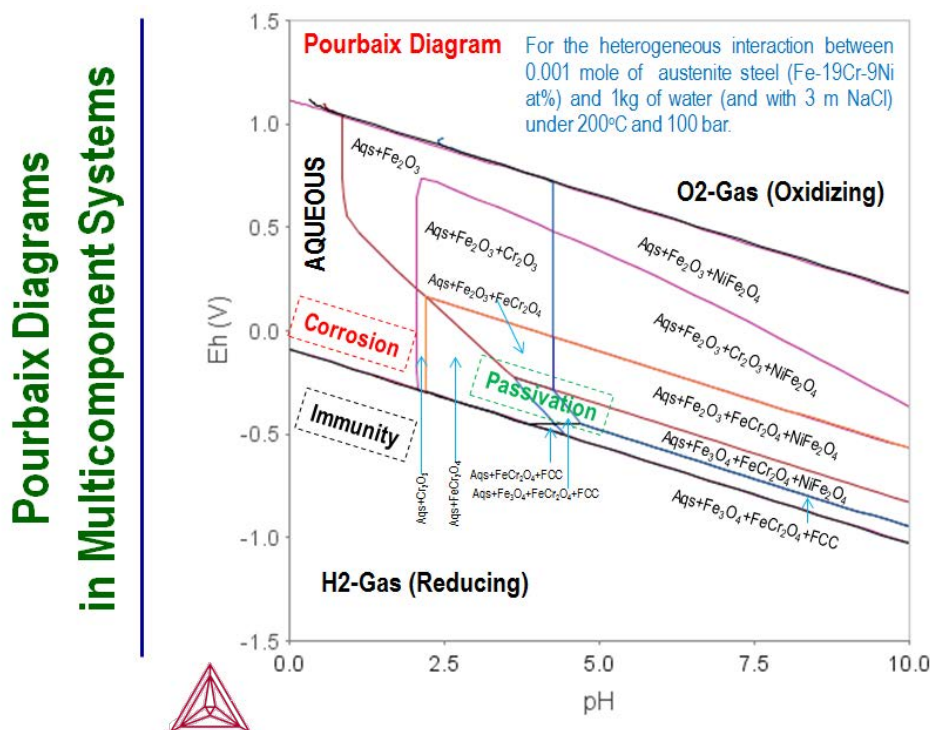
A Pourbaix diagram is a kind of phase diagram that shows the stability boundaries for a metal-aqueous interaction system. The phase boundaries are shown as a function of pH (acidity) and Eh (standard hydrogen electronic potential). An aqueous solution phase is always present in such a system. At a given pH and Eh, a metal may lose its stability to a soluble or corrosive aqueous solution, or be in equilibrium with either the aqueous solution (insoluble/immune) or with a secondary-phase file that has formed (consisting of oxides, hydroxides, sulphides or other solids). In the latter case, further dissolution of the passive or protective metal is prevented.

The speciation and partition in the aqueous solution and the interacting phases depend not only on pH and Eh, but also on other factors such as the bulk composition, temperature and pressure in the system. The interacting phases may be gas mixtures, stoichiometric solids or solid solutions.

A Pourbaix diagram is divided in regions of *immunity*, *corrosion* and *passivity*. These regions provides information about the stability of a particular metal or alloy in a specific aqueous electrochemical environment under certain pH, Eh, pressure and temperature conditions.

- The immunity region is the region in which there is no metal dissolution.
- The corrosion region is the region in which there is active metal dissolution.
- The passivation region is the region in which a protective metal-oxide film that prevents metal dissolution is formed.

The following shows these three regions in a Pourbaix diagram for the heterogeneous interaction between 0.001 mole of austenite steel (Fe-19Cr-9Ni [at%]) and 1 kg of water (with 3 m NaCl), at 200° C and 100 bar:



Depending on the system's bulk chemical composition, secondary phases may form during the transformation process. These can not only be oxides, but also be, for example, hydroxides, sulphides, sulphates, carbonates, nitrates, phosphates, borates, silicates, hydrous silicates and halides. Information about these secondary phases may help one understand the passivation behaviours in corrosion processes. For example, it may be important to understand whether any secondary phases are formed in different pH-Eh regions during hydrolysis, oxidation, reduction or other reaction processes.

In a Pourbaix diagram, the predominant ion boundaries are often represented by dashed and straight lines imposed on a traditional Pourbaix diagram for a simple interaction system (Pourbaix, 1973, 1974; Cramer and Covino, 2003; Verink, 2011; Thompson et al., 2011). Such a predominance boundary is normally an equal molality (or equal activity) line for a pair of two most-concentrated aqueous solute species (charged or neutral) involving a common metal. A line is then simply determined by a reaction constant of its corresponding electrochemical reaction in the homogeneous aqueous solution phase. However, this is not the case in Thermo-Calc.



You cannot get any information about predominant ion boundaries from a Pourbaix diagram in Thermo-Calc.

Working with Pourbaix Diagrams

With the Thermo-Calc software package, Pourbaix diagrams can be calculated over a wide range of pressure, temperature and composition conditions for complex heterogeneous interactions between multicomponent primary alloy solution or compound phases, concentrated aqueous solutions (with dissolved inorganic and organic substances), complicated secondary solids and oxidizing/reducing gaseous mixtures. In the Console Mode, diagrams can be calculated and plotted either using the response-driven POURBAIX module or directly using the DATA, GIBBS, POLY and POST modules.



This command or module is not available with GES6.



GES6 is a re-write and new implementation of the Gibbs Energy System module of Thermo-Calc and it is the default engine. The previous version, GES5, is still available and will continue to work in the background of the program where necessary. The main purpose of GES6 is to support faster development of new features. However, not all GES5 functionality is implemented in GES6. In such cases (except for optimization, PARROT and the POURBAIX module), GES6 falls back silently and uses functionality from GES5 in the background.

It is possible in Thermo-Calc to set aqueous properties other than pH and Eh as axis variables. For example, the following properties can also be set as axis variables: A_h (electronic affinity), p_e (electronic activity $\log_{10} A_{Cr}$), I_S (ionic strength), T_M (total aqueous concentration, in molality), O_C (Osmotic coefficient), activity or activity coefficient of solvent H₂O, and activities or activity coefficients or concentrations in m (molality) of charged or neutral solute species.

Beside a concentrated aqueous solution phase handled by a proper thermodynamic model named SIT, HKF or PITZ, it is also possible to consider complex alloy solution phases or compound phases, as well as secondary solid phases and gaseous mixtures, which are treated by specific solution models.

Most frequently, a Pourbaix diagram is calculated for a specific alloyed phase with the initial alloying composition, such as the FCC solution phase in an austenite steel. However, it is possible to calculate a Pourbaix diagram for two co-existing phases, such as the FCC+BCC solution phases in a duplex steel for example, or even for more than two co-existing phases in a steel/alloy.



Each point on the line in a pH-Eh diagram in Thermo-Calc represents a certain minimum state of Gibbs energy. When a line is crossed, a phase transformation should occur. This means that a Pourbaix diagram in Thermo-Calc does not provide any information about any predominant ion boundary.

Key Concepts

The following are two key concepts important for understanding how aqueous solutions behave and how an aqueous-bearing heterogeneous interaction system is properly defined and calculated in Thermo-Calc.

Effective Interaction Ratio

A pH-Eh plot is always related to a certain amount of initial alloys or other condensed materials that has effectively reacted with an aqueous solution in the system. This is the amount of condensed material that is fully in equilibrium with the defined aqueous solution phase. The amount is specified relative to an aqueous solution that is normally comprised of 1 kg of water with certain specified solute concentrations at certain temperature and pressure conditions. (This is why a calculated Pourbaix diagram is typically presented for an initial amount of the interacting metal or alloy at a certain level, such as 10^{-6} , 10^{-3} , 0.1 or 1 mole of metal or alloy.) It is called the *Effective Interaction Ratio* (between the initial alloy or alloyed phases and the initial aqueous solution) and it is expressed in terms of molality (mol/kg).

The Effective Interaction Ratio is important for two reasons. First, the ratio has implications for kinetic or dynamic effects such as chemical reaction mechanism and kinetics, fluid flow dynamics, surface area and interaction time. Secondly, the ratio, being expressed as 10^{-6} mole of metal (or alloy), is the solubility limit that can be detected for cathodic corrosion protection by immunity.

One should always be careful when setting initial amounts and compositions in the original condensed materials, as well as when setting the initial concentrations of dissolved solutes in the original aqueous solution phase. It is often useful to make a series of calculations for different levels of initial amount of the interacting metal/alloy while the conditions are fixed for other settings (such as initial aqueous concentration, pressure, temperature, pH, and Eh).

Solubility

When a heterogeneous equilibrium has a dissolving solution or mixture phase and a stoichiometric or solution phase, then the concept of solubility becomes important. A solubility of a phase (the solute) is its property of dissolving in the solvent phase. This concept concerns the constitution of a phase and is applied where one or several of the constituents are dominant (which is highly concentrated and dissolving) while there are only small amounts of the other remaining species (which are less concentrated and dissolved). The dissolving solution or mixture phase can be liquid, gas, aqueous or solid, as long as it has dissolving capacity. The stoichiometric or solution phase has some constituents which tend to be dissolved into the dissolving solution or mixture phase.

KEY POINTS ABOUT SOLUBILITY

- Under certain temperature, pressure and composition conditions, a Fe- or Cr-dominant BCC phase can dissolve certain amounts of Ni and C from a carbide phase such as M_23C_6 , M_7C_3 or M_3C . The Ni and C elements in the carbides have the solubility defined relative to the BCC phase.
- An aqueous solution phase is always dominant in the solvent water, that is, H_2O . Under specific temperature, pressure and aqueous composition conditions, any other element (such as Fe and C) or substance (such as a pure SO_2 gas, stoichiometric phase Cu_2S and solution phase $(Fe,Ni)_1(O,Va)_1$) have a certain solubility limit in the defined aqueous solution.
- Under certain temperature and pressure conditions, and under given certain concentrations of other dissolved species in the mixture, an O_2 -dominant gaseous mixture phase can dissolve certain amounts of Fe^{+2} or Fe^{+3} species from magnetite (Fe_3O_4). The magnetite solid has solubility defined relative to the gaseous mixture under the given conditions.
- Under certain temperature and pressure condition, under specific concentrations of other dissolved species in the liquid phase, a Fe-dominant liquid mixture phase can dissolve certain amounts of, for example, Cr and O. The Cr and O components have the solubility defined in the liquid mixture.

Basic Settings and Definitions

In a homogeneous aqueous solution or an aqueous-bearing heterogeneous interaction system, the most essential definition is for system-components there must be H_2O , H^{+1} and ZE (electron) plus those for elements dissolved in aqueous solution (such as Na , Cl , S) and associated in interacting metals/alloys (such as Fe , Cr , Mn , Mg , Ni , Al , Si , Zn). Three fundamental phases in a system are the `AQUEOUS` solution, the `GAS` mixture and the `REF_ELECTRODE`. The `REF_ELECTRODE` phase is used for setting the reference state for electrostatic potential in the system and for calculating the Eh condition (defined as $MUR(ZE) / RNF$). Other phases should be appropriately selected and retrieved from critically-assessed databases that cover not only the target phases (solution or stoichiometric) in interacting metals/alloys but also the secondary phases (solution or stoichiometric). The two public databases PAQ and PAQS are specially designed as single-database choices that cover all kinds of phases necessary for calculations. However, these databases are each limited to a framework of a very small number of elements. When it comes to simulations of complex multicomponent systems with a wide variety of elements and phases, the thermodynamic data must be selected and retrieved from several databases: `AQUEOUS` solution and `REF_ELECTRODE` phases must be retrieved from TCAQ or AQS; alloy phases (such as `FCC_A1`, `BCC_A2`, `HCP_A3`, `CEMENTITE`) from alloy solution databases (such as SSOL for general alloy phases, TCFE for steel/Fe-alloy phases, TCAL for Al-based alloy phases; TCMG for Mg-based

alloy phases, and TCNI for Ni-based superalloy phases); gaseous mixture phase and secondary phases from specific substance or solution databases (such as SSUB for GAS phase and various solid compound phases or TCOX for oxide solution phases). Note that the REF_ELECTRODE phase should always be suspended in equilibrium calculations, while GAS phase could be set as ENTERED, SUSPENDED or DORMANT, depending on the purpose of the calculation.

When defining an interaction system, the initial condition for the H₂O component is always set as 1 kg of water. The initial composition conditions for dissolving and interacting elements are normally defined in moles (such as $n(\text{Fe})=0.009$, $n(\text{Cr})=5\text{E}-4$, $n(\text{Ni})=3\text{E}-4$, $n(\text{Mn})=5\text{E}-5$, $n(\text{S})=5\text{E}-5$, $n(\text{Na})=3$, $n(\text{Cl})=3$). This makes it straightforward and convenient to count various related aqueous solution properties based on molality. The initial conditions for the H+1 and ZE components can be given as molar compositions (such as $n(\text{H}+1)=0$, $n(\text{ZE})=0$) or their activities or potentials (such as $\ln \text{ACR}(\text{H}+1)=-9.21$, $\text{MUR}(\text{ZE})=8400$).

The pH and Eh properties of the aqueous solution in the interacting system are always defined in the following way:

$$\text{pH} = -\log_{10}[\text{ACR}(\text{H}+1, \text{AQUEOUS}) * \text{AH}_2\text{O}] \quad \text{Eh} = \text{MUR}(\text{ZE}) / \text{RNF}$$

The symbol AH₂O is the molecular weight of solvent H₂O (equals 55.508435) and RNF is the Faraday constant (equals 96485.309).

The activity of the solvent water (ACRH₂O, A_w), the osmotic coefficient of aqueous solution (OSMC, O_s), electronic affinity (A_h), electronic activity log₁₀ACRe (p_e), ionic strength (IS), total aqueous concentration, in molality (T_M) and total alkaline concentrations under two definitions (A_{t1}/A_{t2}) are calculated and listed for each equilibrium state.

POLY3 calculations for mass balances in Thermo-Calc are always based on site-fractions. Consequently, when functions for describing various properties of aqueous solutes are defined, such as molality (ML_i), activity coefficient (RC_i) and activity (AI_i), they should be converted to molality-based quantities:

$$\begin{aligned} \text{ML}_i &= Y(\text{AQUEOUS}, i) * \text{AH}_2\text{O} / \text{YH}_2\text{O} \\ \text{RC}_i &= \text{ACR}(i, \text{AQUEOUS}) * \text{YH}_2\text{O} / Y(\text{AQUEOUS}, i) \\ \text{AI}_i &= \text{ACR}(i, \text{AQUEOUS}) * \text{AH}_2\text{O} \end{aligned}$$

Here, YH₂O is the site-fraction of solvent H₂O and AH₂O equals 55.508435.

Many more variables, functions and tables can be entered for various purposes. For instance, an equilibrium constant for a homogeneous reaction or a solubility product for a solid dissolution reaction can be entered.

Thermodynamic Data Requirements

In this section:

| | |
|--------------------------------------------|----|
| Required Thermodynamic Data | 12 |
| Including or Excluding the Gas Phase | 12 |

Required Thermodynamic Data

To calculate a Pourbaix diagram, thermodynamic data for at least the following four types of phases must be available:

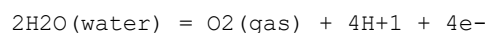
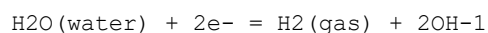
- The aqueous solution phase which applies a certain aqueous solution model. In Thermo-Calc, information about this phase could be retrieved from, for instance, the TCAQ or AQS database (these also include data for the `REF_ELECTRODE` phase that is used for setting the reference state of the standard hydrogen electrode).
- The alloy solution and/or compound phases for the primary matrix phases (and possibly also for the precipitated phases in the alloy. Examples of such phases include FCC_A1, BCC_A2, HCP_A3, SIGMA and CEMENTITE. In Thermo-Calc, information about such phases could be retrieved from, for example, the TCFE database for steels/Fe-alloys, the TCNI database for Ni-based superalloys, the TCAL database for Al-based alloys, the TCMG database for Mg-based alloys, the TCSLD for Sn-/Au-/Bi-/Zn-based solder alloys or the SSOL for general alloys.
- The secondary solid phases that would form as a result of the heterogeneous chemical or electrochemical reactions. These phases could be, for example, oxides, hydroxides, silicates, hydrous silicates, sulphides, sulphates, carbonates, nitrates, phosphates, borates or halides. In Thermo-Calc, information about such phases could be retrieved from, for example, the SSUB database for pure solid compounds or the TCOX database for complex oxide solids.
- The gaseous mixture phase. Information about this phase could be retrieved from, for example, the SSUB database. However, note that it is also possible to perform Pourbaix diagram calculations that ignore the gaseous mixture phase.

All this thermodynamic data about the various phases must be critically assessed and internally consistent. Furthermore, when the data is retrieved from several databases, the data taken from each database must be consistent with the data taken from the other databases. When Pourbaix diagrams and other diagrams of steel corrosion processes are calculated, it is typically recommended that the TCAQ, TCFE, SSUB and TCOX databases or the AQS, TCFE, SSUB and TCOX are used in combination.

The public PAQ database contains thermodynamic data for all four phase types and can be used for calculating Pourbaix diagrams. They have been designed specifically for the purpose of demonstrating the POURBAIX module functionality in Thermo-Calc. However, these databases only allow you to perform test calculations for simple cases with major phases in which only a few elements can be considered.

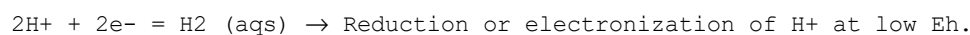
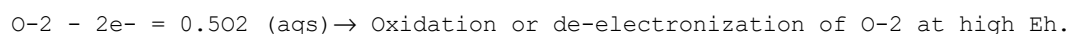
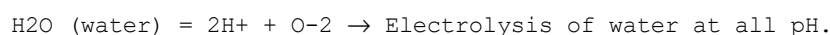
Including or Excluding the Gas Phase

Under defined pressure and temperature conditions, the solvent water's thermodynamic stability limits are determined by the following two electrochemical reactions:

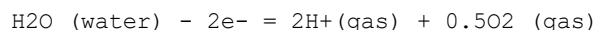
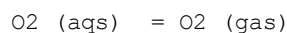


The first reaction describes the formation of H₂-dominated gaseous mixture, under reducing conditions. The second reaction describes the formation of O₂-dominated gaseous mixture, under oxidising conditions.

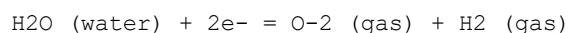
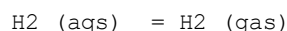
If the system reaches global equilibrium, then the water component is electrolyzed to H⁺ and O²⁻ at all pH conditions. The degree of electrolysis depends on the pH value in the aqueous solution phase. If Eh gets high enough, then the O²⁻ anion is oxidized to O₂ (aq). On the other hand, if Eh gets low enough, then the H⁺ cation is reduced to H₂ (aq). The major electrolysis and redox reactions are the following:



At a critically high Eh value under a given pH condition, an aqueous solution phase with a high enough O₂ activity becomes less stable than an O₂-dominated gaseous mixture phase. At this point, the gas phase replaces the aqueous solution phase in the system. The replacement process can be characterised by the following phase-transformation on the aqueous-gas phase boundary and oxidation of remaining water:



Similarly, at a critically low Eh value under a given pH condition, an aqueous solution phase with a high enough H₂ activity becomes less stable than a H₂-dominated gaseous mixture phase. At this point, the gas phase replaces the aqueous solution phase in the system, through the following phase-transformation on the aqueous-gas phase boundary and reduction of remaining water:



The phase transformation from an aqueous solution phase to an O₂- or H₂-dominated gaseous mixture phase also depends on the total molar Gibbs energies of the phases (which are complex functions of the phase constituents, the temperature and the pressure). The Gibbs energy minimization technique used in Thermo-Calc ensures that the phase transformation is accurately simulated.

The following Pourbaix diagrams show the result of a calculation where the gaseous mixture phase was included. In the upper region (high Eh) and lower region (low Eh), the aqueous solution phase has been oxidized and reduced, respectively, to an O₂- or H₂-dominated gaseous mixture phase.

The two example diagrams show that the upper and lower boundaries between the aqueous phase (water) and the gas phase (dominated by either O₂ or H₂) can shift when solutes dissolve or when the temperature and pressure change.

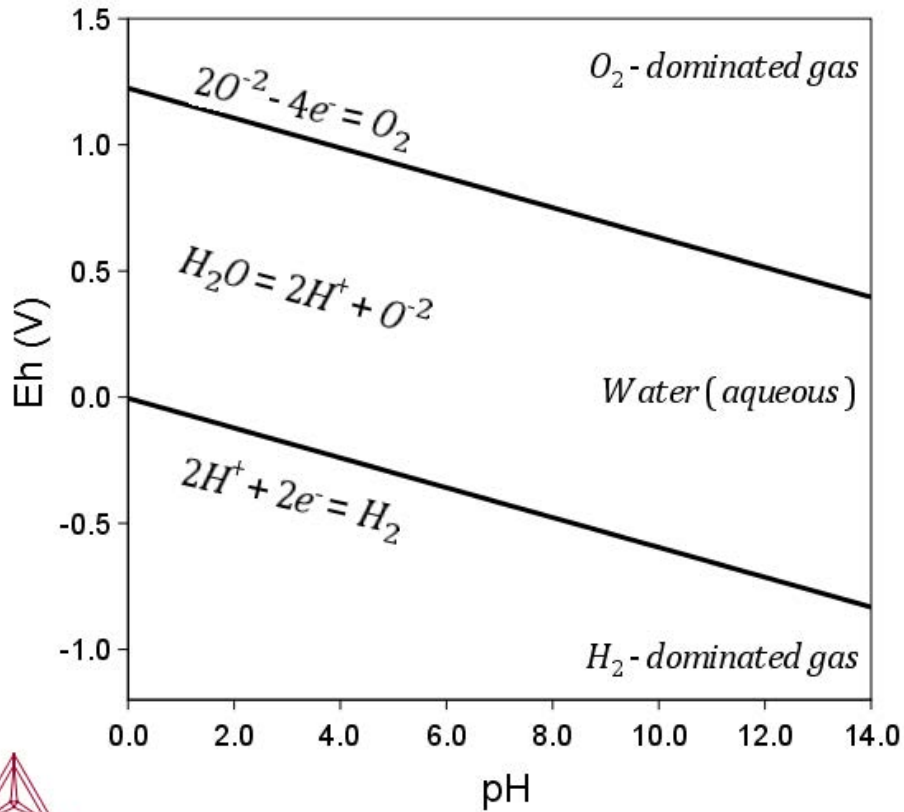
Accordingly, if one does not take a gaseous mixture phase into account when performing a calculation of Pourbaix diagram (as above), then the aqueous solution phase may end up with an extremely high O₂ (aq) concentration at high Eh condition, or an extremely high H₂ (aq) concentration at low Eh condition. Under either of these two extreme circumstances, the concept of “aqueous solution phase” is no longer valid and consequently no proper aqueous solution model can actually be applied. Therefore, from a restrictive thermodynamic equilibrium point of view, one shall normally include a gaseous mixture phase in an aqueous-bearing heterogeneous interaction system. This is true for all types of equilibrium calculations for an aqueous-bearing heterogeneous interaction system, not only of Pourbaix diagram calculations.

Hence, to perform a completely accurate Pourbaix diagram calculation, the gaseous mixture phase must be taken into account. However, since these electrochemical reactions normally have much higher kinetic barriers and are slower than other electrochemical and chemical reactions in the interaction system, one can sometimes ignore the gaseous mixture phase in the calculation. Note that if the gaseous mixture phase is ignored in this way, then the Pourbaix diagram does not show the H₂O-stability limiting lines.

EXAMPLE DIAGRAMS

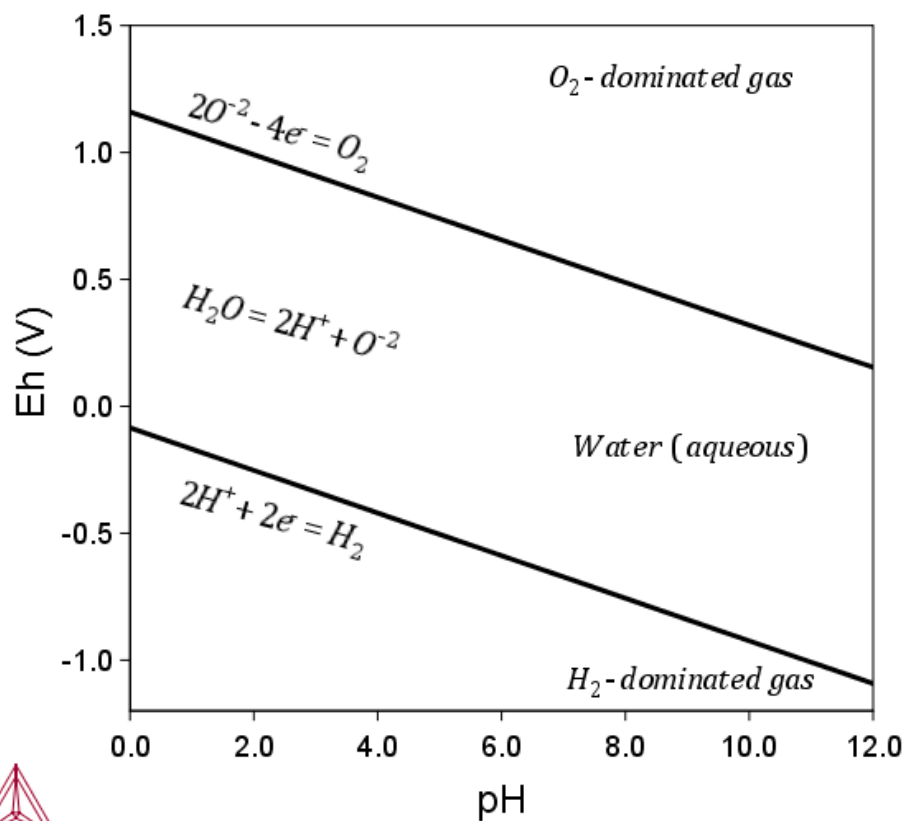
The first diagram is a pH-Eh diagram for pure water at 25° C and 1 bar:

Pure water at 25 °C and 1 bar



The second diagram is a pH-Eh diagram for 3mNaCl-0.001mCO₂-0.001mSO₂ aqueous solution at 150° C and 100 bar.

3mNaCl-0.001mCO2-0.001mSO2 aqueous, 150 °C and 100 bar



Examples of Pourbaix Diagrams for Fe

The following two topics are examples of Pourbaix diagrams for Fe. For the first example, the calculations on which the diagrams are based have not taken the gas phase into account. The diagrams in the second example are based on calculations that have taken the gas phase into account.

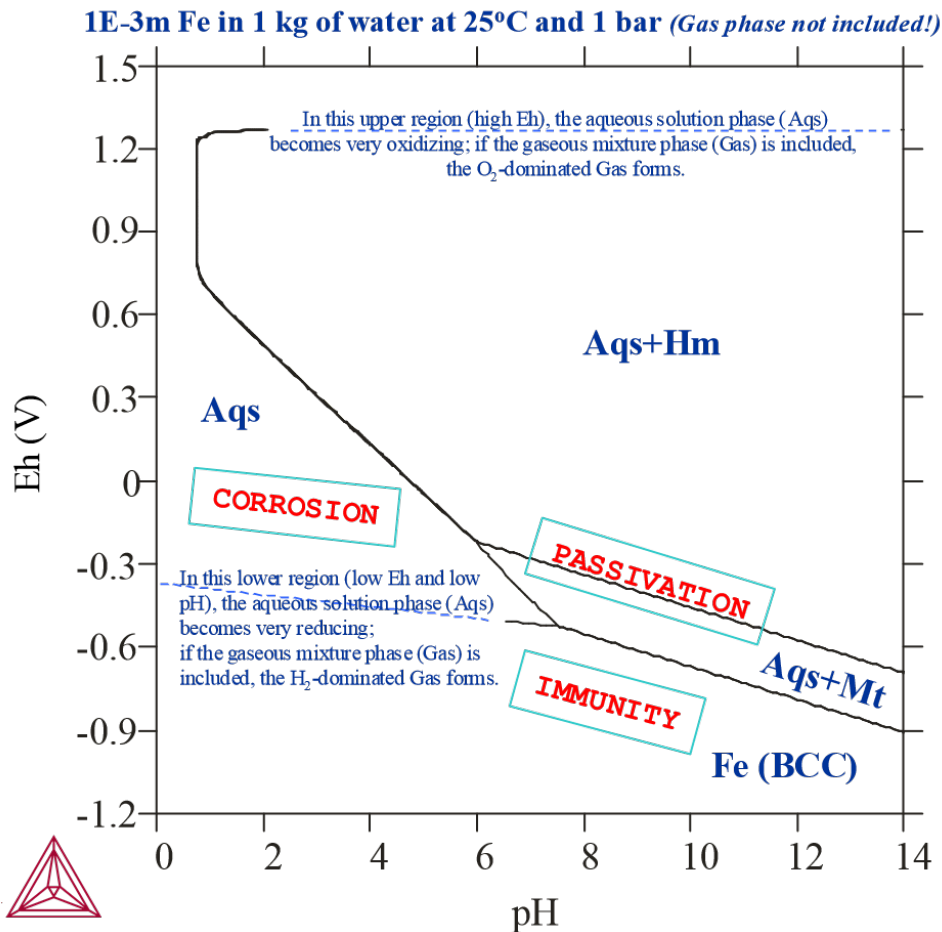
In this section:

| | |
|-------------------------------------------------|----|
| Pourbaix Diagrams with Gas Phase Excluded | 18 |
| Pourbaix Diagrams with Gas Phase Included | 18 |

Pourbaix Diagrams with Gas Phase Excluded

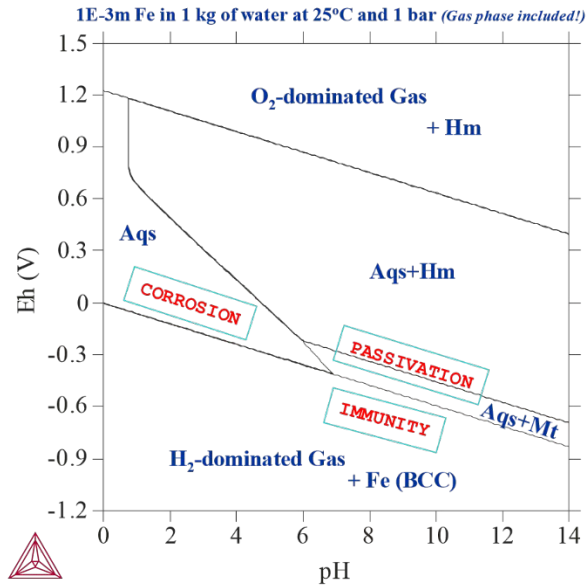
This is an example of a Pourbaix diagram of Fe, in which the gas phase has not been considered in the calculation. The system has 0.001 mole of Fe in 1 kg of pure water at a temperature of 25°C and a pressure of 1 bar. Magnetite (Mt, Fe_3O_4) and hematite (Hm, Fe_2O_3) co-exist with the Fe-containing dilute aqueous solution. The formation of magnetite and hematite represent the passivation of iron in the upper right pH-Eh field.

If pH is low and Eh is relatively high, then Fe eventually completely dissolves into the aqueous solution phase. Under conditions of low Eh, Fe remains in its stable solid state, the BCC phase, and neither dissolves into water nor into alternates to Fe (the immunity of Fe).



Pourbaix Diagrams with Gas Phase Included

With all the possible redox reactions involving the aqueous solution phase and gaseous mixture phase being considered in the equilibrium system, that is, the gaseous mixture phase is included in the calculation, the Pourbaix diagram of Fe in a system with 0.001 mole of Fe in 1 kg of pure water at 25°C and 1 bar.



Comparing this Pourbaix diagram with that from ["Basic Settings and Definitions" on page 9](#), you can see that both diagrams are for the same interaction system under the same temperature-pressure condition, but the present diagram shows the results of calculations where the gaseous mixture phase has been included. It presents the complete Pourbaix diagram for the defined interaction system, in a full thermodynamic equilibrium. In the upper region (high Eh) and lower region (low Eh), the aqueous solution phase is oxidised and reduced to the O₂- or H₂-dominated gas phase. Hematite coexists with the O₂-dominated gas, while Fe-BCC is stable with the H₂-dominated gas. The stability field of magnetite may extend slightly into the H₂-dominated gas region, where it coexists with the gaseous mixture instead of the aqueous solution. Its boundary with Fe (BCC) cannot be drawn due to the absence of aqueous solution phase.

It is not possible to calculate the pH value in both the O₂- and H₂-dominated gaseous mixture phase stability regions where the aqueous solution phase is absent. Hence, in a normal Pourbaix diagram, no line is drawn that indicates a phase boundary between the gas phase and the metallic phases or secondary phases (that is, metal-oxides).

Other Examples of Pourbaix Diagrams

In this section:

| | |
|--------------------------------------------|----|
| Variations of Pourbaix Diagrams | 21 |
| Pourbaix Diagrams for Complex Alloys | 23 |

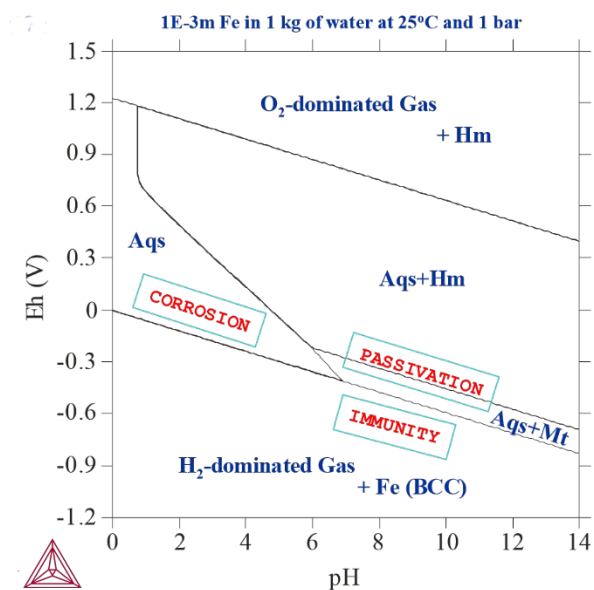
Variations of Pourbaix Diagrams

The shape of a Pourbaix diagram of an alloy or condensed material and the stability relations of various secondary phases depend upon the following system factors:

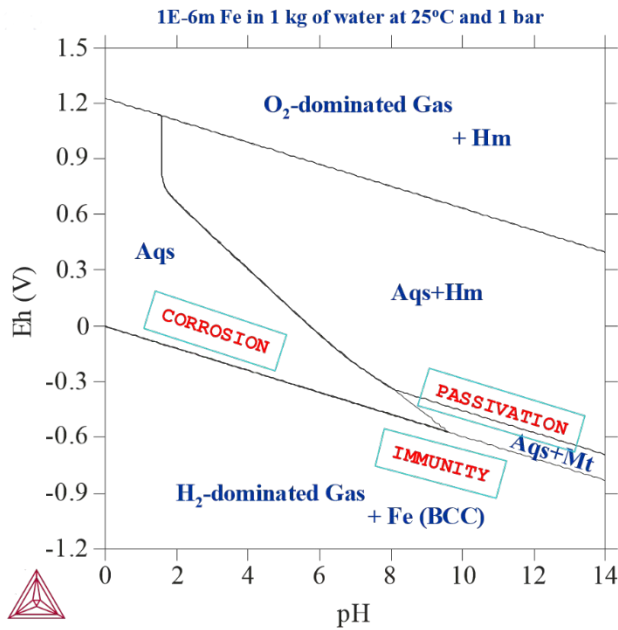
- Initial amount of the alloy or other condensed materials
- Initial composition of the alloy or other condensed materials
- Initial amount of the interacting aqueous solution phase
- Initial composition of the interacting aqueous solution phase
- Temperature and pressure conditions

In the interaction system that the diagrams in ["Pourbaix Diagrams with Gas Phase Excluded" on page 18](#) and ["Pourbaix Diagrams with Gas Phase Included" on page 18](#) are based on, the initial amount of pure Fe that was taken to have effectively reacted with 1 kg of pure water at 25° C and 1 bar was 0.001 m. The following diagrams are Pourbaix diagrams of Fe where other initial amounts of pure Fe have been used, or where the interacting aqueous solution compositions have been alternated, or the temperature and/or pressure have been changed. Gaseous mixture phases have been included in all the calculations that these diagrams are based on.

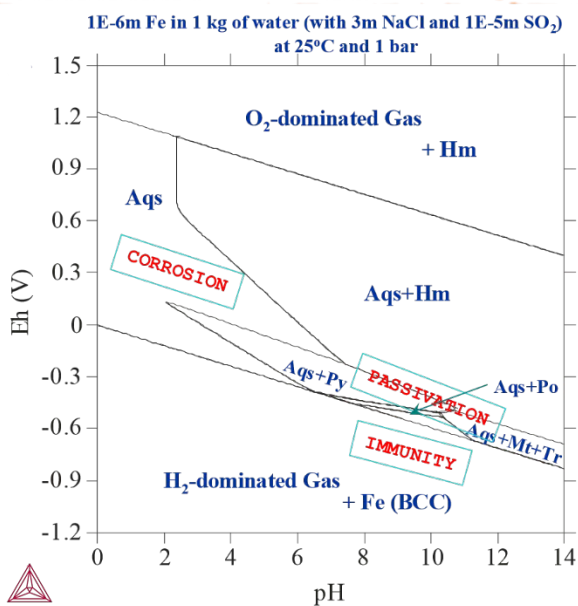
In the first diagram, 1E-3 m Fe actively reacted with 1 kg of pure water at 25° C and 1 bar (as in the calculation in Pourbaix Diagrams with Gas Phase Included):



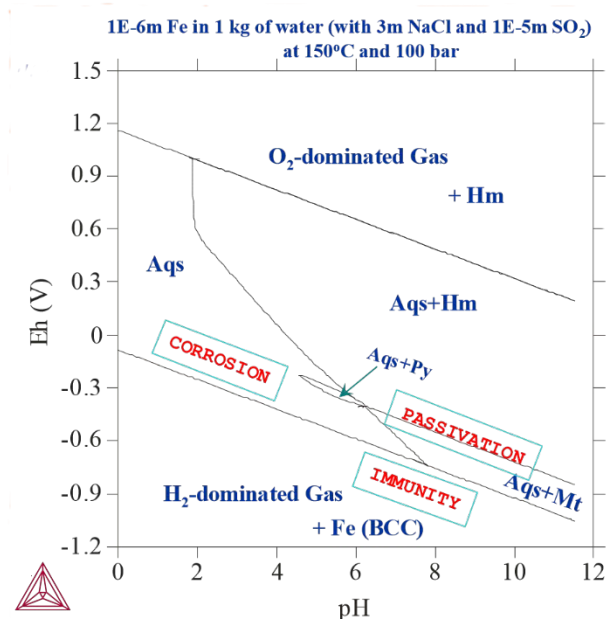
In the second diagram, 1E-6 m Fe actively reacted with 1 kg of pure water at 25° C and 1 bar. Note that the active metal corrosion region gets enlarged as the initial Fe amount decreases from 1E-3m to 1E-6m:



In the third diagram, 1E-6 m Fe actively reacted with 1 kg of water, 3m NaCl and 1E-5 m SO₂ at 25° C and 1 bar. Introducing SO₂ into the system leads to the formation of various metal-sulphides (Py-pyrite, Popyrrhotite, Tr-troilite). In addition, the passivation region becomes larger.



Finally, in the fourth diagram, 1E-6 m Fe actively reacted with 1 kg of water, 3m NaCl and 1E-5 m SO₂ at 150° C and 100 bar. Here, changing the temperature and pressure affects the stability fields of various Fe-oxides/sulphides.

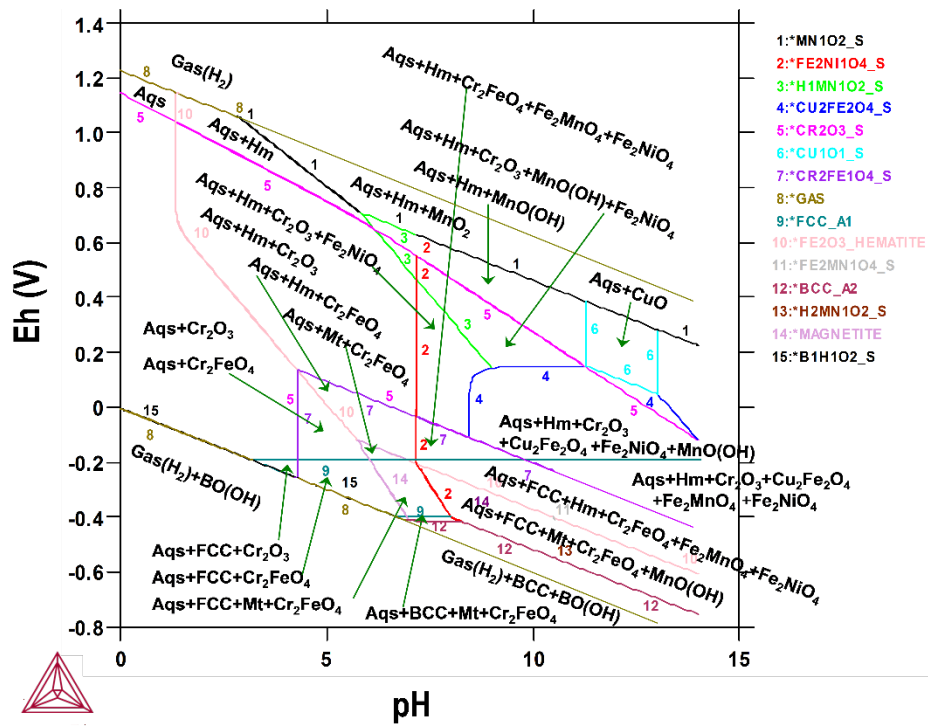


As you can see from the four diagrams, the aqueous-gas phase boundaries shift as the initial bulk compositions, pressure and temperature conditions in the interaction system change.

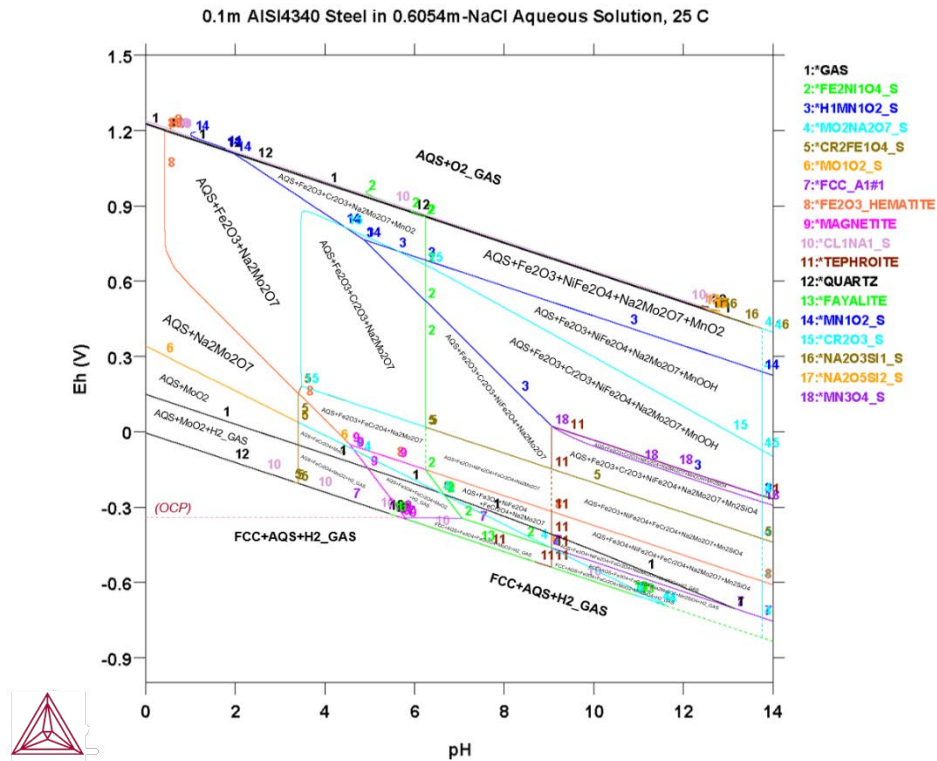
Pourbaix Diagrams for Complex Alloys

Thermo-Calc can not only be used to simulate how pure metals interact with pure water or simple aqueous solutions under normal pressure and temperature conditions. It can also be used to calculate how complex alloys and concentrated aqueous solutions interact over a very wide pressure, temperature and composition ranges. This is illustrated with the two examples.

The first example is a Pourbaix diagram calculated for the heterogeneous interaction between 0.001 mole of steel (Fe-7.676Cr-5.0Ni-2.1887Mn-1.0Cu [at%]) and 1 kg of water (and with 1.2 m H₃BO₃, 0.022 m Li and 0.001 m NH₃), at 25° C and 1 bar. This application is particularly useful for safety assessments of nuclear reactors and nuclear waste repositories.



The next example is a Pourbaix diagram calculated for the heterogeneous interaction systems between 0.1 mole of AISI4340 stainless steel (Fe-0.80Cr-1.85Ni-0.70Mn-0.25Mo-0.25Si-0.40C [wt%]) and 1 kg of seawater (with the equivalent of 0.6054 m NaCl), at 25° C and 1 bar. This application is particularly useful for failure analysis of petroleum exploitation industry.



Pourbaix Diagram References

1. Andersson J-O., Helander T., Höglund L., Shi P., and Sundman B. (2002). Thermo-Calc and DICTRA, Computational tools for materials science. *Calphad*, 26: 273-312.
2. Ciavatta, L. (1990). The specific interaction theory in equilibrium analysis. Some empirical rules for estimating interaction coefficients of metal ion complexes. *Ann Chim. (Rome)*, 80, 255-263.
3. Cramer, S.D. and Covino, B.S. Jr. (2003). *Corrosion: Fundamentals, Testing, and Protection*. ASM Handbook, Volume 13A.
4. Helgeson, H.C., Kirkham, D.H., and Flowers, G.C. (1981). Theoretical prediction of the thermodynamic behavior of aqueous electrolytes at high pressures and temperatures: IV. Calculation of activity coefficients, osmotic coefficients, and apparent molal and standard and relative partial molal properties to 600° C and 5 kb. *Am. J. Sci.*, 281, 1249- 1516.
5. Johnson, J.M. and Norton, D. (1991). Critical phenomena in hydrothermal system: State, thermodynamic, electrostatic, and transport properties of H₂O in the critical region. *Am. J. Sci.*, 291, 541-648.
6. Kaufman, L. (2002). Calculation of Pourbaix diagrams for C22 in various well water chemistries. In: *Proceedings for the 5th Nickel Development Institute Workshop on*

Fabrication of Welding of Nickel Alloys (R. Moeller, ed.), Nickel Development Institute, Las Vegas, Nevada, 16-17 Oct., 2002.

7. Kaufman, L., Perepezko, J.H., Hildal, K., Farmer, J., Day, D., Yang, N., and Branagan, D. (2009). Transformation, stability and Pourbaix diagrams of high performance corrosion resistant (HPCRM) alloys. *Calphad*, 33: 89-99.
8. Pourbaix, M. (1973). *Lectures on Electrochemical Corrosion*. Plenum Press, New York.
9. Pourbaix, M. (1974). *Atlas of Electrochemical Equilibria in Aqueous Solutions, 2nd Ed*, Houston, Tex., National Association of Corrosion Engineers.
10. Shi, P. (2013a). *Thermo-Calc 3.0 (Console Mode) Manual* (including *TC3-CM User's Guide*, and *Thermo-Calc Software System*), Thermo-Calc Software, Stockholm, Sweden.
11. Shi, P. (2013b). *Materials Corrosion Applications with Thermo-Calc Software*. Thermo-Calc Software, Stockholm, Sweden.
12. Shi Pingfang, Engström A, and Sundman B (2011a). Thermodynamic investigations on materials corrosion in some industrial and environmental processes. *Journal of Environmental Sciences*, 23 (Supplement): S1-S7.
13. Shi, P., Engström, A., Sundman, B., and Ågren, J. (2011b). Thermodynamic calculations and kinetic simulations of some advanced materials. *Materials Science Forum*, 675-677: 961-974.
14. Thompson, W.T., Kaye, M.H., Bale, C.W., and Pelton, A.D. (2011). Pourbaix diagrams for multielement systems. In: *Uhlig's Corrosion Handbook, 3rd Edition* (Revie RW, Ed.), The Electrochemical Society and Jon Wiley & Sons, New Jersey.
15. Verink, E.D. (2011). Simplified procedure for constructing Pourbaix diagrams. In: *Uhlig's Corrosion Handbook, 3rd Edition* (Revie RW, Ed.), The Electrochemical Society and Jon Wiley & Sons, New Jersey.