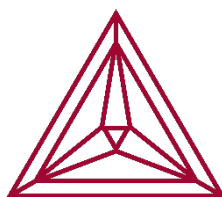




Thermo-Calc User Guide

Version 2015b



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2. Introduction to Thermo-Calc

This guide is an introduction to working with both *Graphical Mode* and *Console Mode* in Thermo-Calc.

- [The Thermo-Calc Software](#)
- [Typographical Conventions](#)
- [Graphical Mode vs Console Mode](#)
- [Help Resources](#)
- [Example Collections](#)
- [The Thermo-Calc Modules](#)
- [Displaying Thermo-Calc License Information](#)
- [Databases](#)
- [Using This Guide](#)


2.1 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.

A Software Development Kit (SDK) is available. This SDK is used to plug the calculation engine into your own application or into other third-party applications.





The Thermo-Calc program also includes modules to run simulations of diffusion controlled transformations in multicomponent systems, DICTRA and DIC_PARROT.

 For information about how to use DICTRA in Console Mode, search the online help or see the [DICTRA User Guide](#).

2.2 Typographical Conventions

The following conventions are used throughout the documentation:

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 .

<i>Convention</i>	<i>Definition</i>
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.
COMMAND	This font and all capital letters in the body of the text indicates that this is a COMMAND used in the Console Mode terminal. Examples of how you can use a command are written with the <code>code</code> font: SET_CONDITION T=1000 P=1E5 X(C)=0.01 N=1
<u>HELP</u>	Text in <u>blue and underline</u> is a link to another section.
<Enter>	Text with <angle brackets> indicates a keyboard entry. Usually to press <Enter> (or Return).
<code>code</code> and code bold	A <code>code</code> font shows a programming code or code example. The code bold font highlights the entry.
Important	 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 to more information.
Also see	 Go to more information about the topic being discussed.
Examples	 Go to the example collection to learn more.

2.3 Graphical Mode vs Console Mode

There are two interfaces for the Thermo-Calc program: *Graphical Mode* with a graphical user interface (GUI) and *Console Mode*, which uses a command line interface.

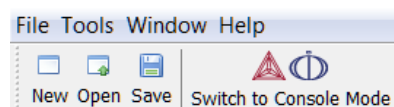
- In Graphical Mode calculations are set up, carried out, and visualized as part of a *project*. The steps in the project are performed with *activities*. There are templates and a Wizard available to guide you through the process of defining the project.

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

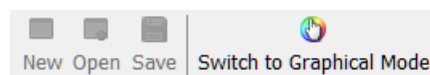
2.3.1 Switching Between Modes

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 toolbar where you switch between modes. The first example is the toolbar in Graphical Mode.



In Console Mode, except for the **Switch to Graphical Mode** button, the toolbar is not used.



👁 Also see [Main Menu and Toolbar](#) for information about the **Tools**, **Window** and **Help** menus, which are available in both modes.

📘 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.

👁 Also see [Graphical and Console Mode-Plotting](#).

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

2.4 Help Resources

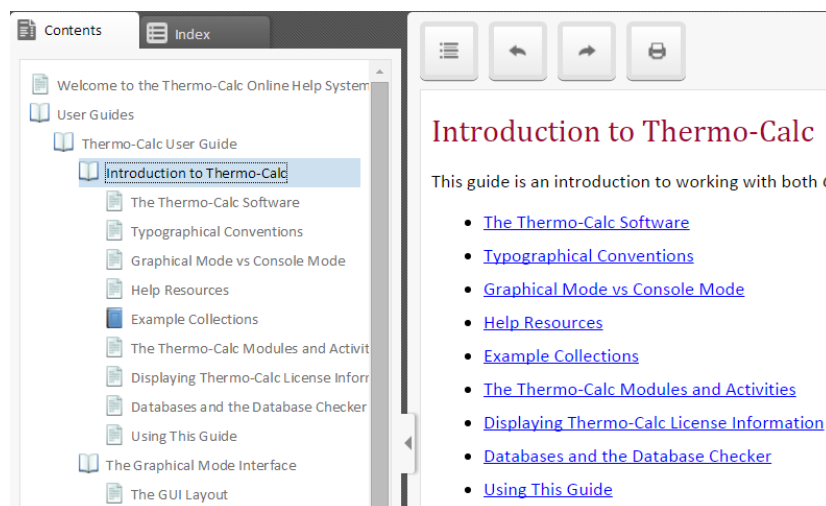
All the documentation and examples are available online or in PDF format.

2.4.1 Using Online Help

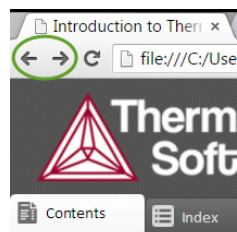
To access online help, open Thermo-Calc and select **Help** → **Online Help**. This online help contains the same documentation that is installed in folders with your software. The advantage is you can browse all the content and search for key words and phrases.

Browse

Use the Contents panel to explore the documentation. Click to expand or collapse a branch in the tree. The node you click in Contents opens the topic in the right panel. In this example, the content is a list of topics. Click the links to go to those topics.

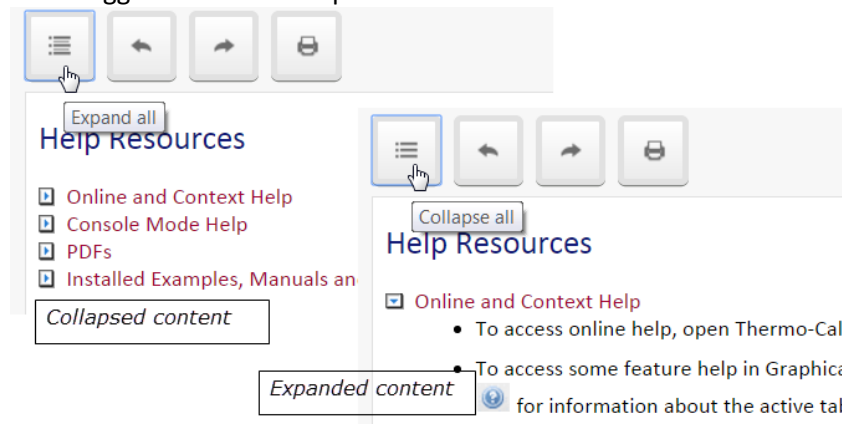


Click the web browser navigation buttons after clicking a link: When you are in the help content and you click a hyperlink, use the web browser buttons to move back and forth in the history.



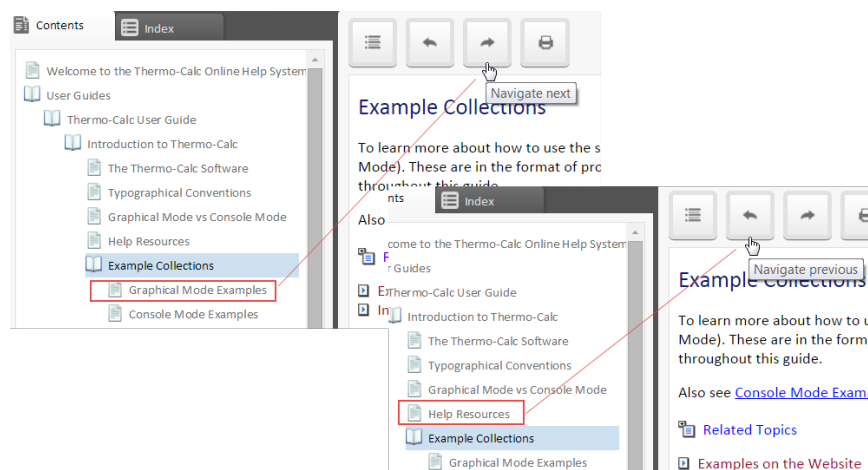
Toggle between Expand All and Collapse All

On pages that have content in drop-down lists, click **Expand all** and **Collapse all** to toggle between the options.



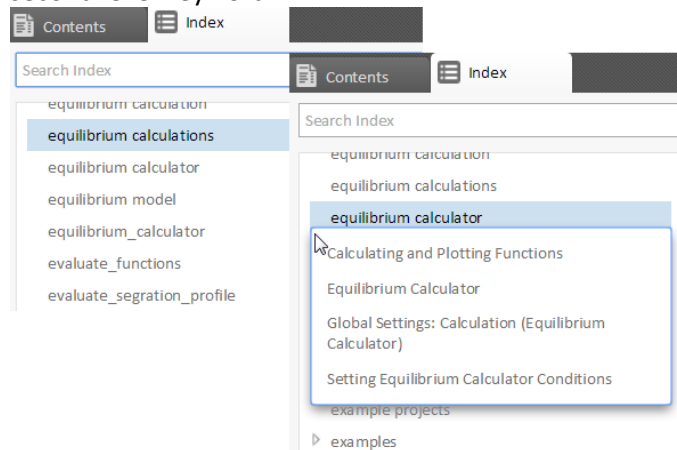
Navigate Previous and Navigate Next

Click the **Navigate previous** or **Navigate next** buttons to move back and forth through the documentation tree one topic at a time.



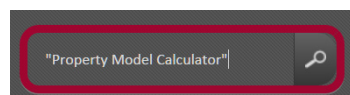
Browse the Index

Click the **Index** tab and scroll through the keyword terms. Click a term to open a list of related topics. Click keywords with an arrow next to them to view the second level keyword.



Search the Contents

Enter a search word or string. To search for a specific phrase or word, enclose it in quotation marks ("). For example, "Property Model Calculator" returns only results with that string but Property Model Calculator searches for all the words.



Your search for "Property Model Calculator" returned 9 result(s).

[Property Model Calculator](#)

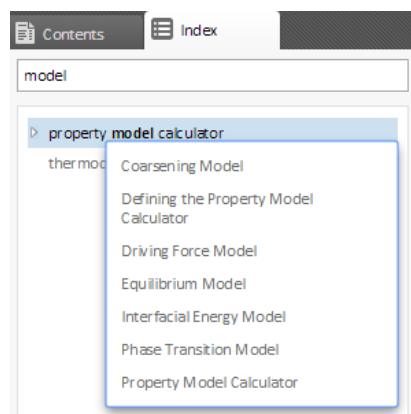
A **Property Model Calculator** allows you to predict and optimize material properties. A set of general models (Model, Interfacial Energy Model, Coarsening Model, and an Equilibrium Model). You can evaluate models sir [User_Guide_-_Thermo-Calc/Property_Model_Calculator.htm](#)

[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 act predecessor. A predecessor is performed before the predecessor's successors and its result is fed forward to : [User_Guide_-_Thermo-Calc/Activity_Successor_and_Predecessor.htm](#)

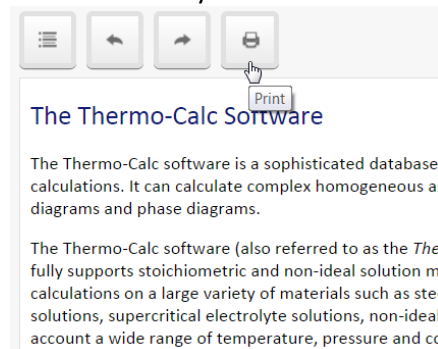
Search the Index

Enter a search word or part of a word. Results are listed. Click a keyword to open a list of related topics.




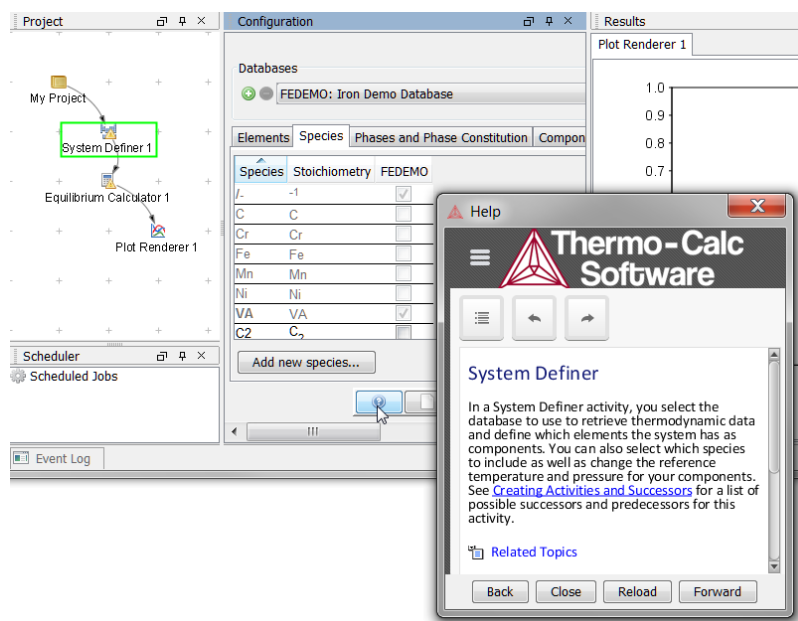
Print

Click the print button to print the content in the right panel. This button is not available when you use the Context help window.




2.4.2 Using Context Help

To access some feature help, in the lower left corner of the Configuration window, click the help button  for information about the active tab or node. In this example, clicking the button opens information about **System Definer**.



The window that opens has the same content as the help you access in the browser except you cannot **Print** from this window.

Click the **Contents**  button to toggle open and close the **Contents** and **Index** tabs as well as Search functionality.

Use the **Collapse all**, **Navigate previous**, and **Navigate next** buttons



to browse the content as described in Welcome to Thermo-Calc.

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.


2.4.3 Console Mode Help

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.

2.4.4 PDFs

On [Thermo-Calc Software's website](#) and wherever the software is installed, folders containing the PDFs versions of the documentation are also downloaded.

 Also see the *Thermo-Calc Installation Guide* for details of where these are installed for your operating system.

2.5 Example Collections

To learn more about how to use the software you can open and run the example projects (Graphical Mode) and macro files (Console Mode). These are in the format of project files (*.TCU) and macro files (*.TCM), respectively. Some examples are referred to throughout this guide.

Examples on the Website

You can find the Graphical and Console Mode examples on the [website](#) under **Examples**. The example files are also included in the installation.

EXAMPLES

Thermo-Calc Graphical Mode

Description of a few selected examples to get started using Graphical Mode in Thermo-Calc

[Thermo-Calc Graphical Mode Examples Guide](#)

[Thermo-Calc Graphical Mode Examples](#)

Thermo-Calc Console Mode

More than 50 examples using Console Mode in Thermo-Calc

[Examples guide](#)


[Example files for Windows](#)


[Example files for Mac and Linux](#)

Figure 1: The Examples available on the Thermo-Calc website.

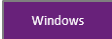

Installed Examples


The default directories where the software and its components are installed, vary by platform and user type.

 On a Windows network user login, the Thermo-Calc and DICTRA Examples and Materials folders are located here **C:\Users\Public\Documents\Thermo-Calc\2015b**. The TC_PRISMA Examples folder is located here **C:\Users\<user>\Documents\Thermo-Calc\2015b**. For all products, the manuals are located here **C:\Program Files\Thermo-Calc\2015b\Manuals**.

 On Windows, once Thermo-Calc is installed, you can also locate the Thermo-Calc and DICTRA Examples and Materials folders, plus all the Manuals using the shortcuts located in the Start menu. Go to **Start → All Programs > Thermo-Calc** and click **Examples**, **Manuals**, or **Materials** as required to open the applicable folder. The TC_PRISMA Examples folder is currently available from here **C:\Users\<user>\Documents\Thermo-Calc\2015b**.













In the table, <user> stands for the username and <version> for the version of Thermo-Calc, for example 2015b.

OS	User type	Default directory
	Normal user	<ul style="list-style-type: none"> Users\<user>\Thermo-Calc\<version> Users\<user>\Documents\Thermo-Calc\<version> My documents
	Administrator	<ul style="list-style-type: none"> Program Files\Thermo-Calc\<version> Users\Public\Documents\Thermo-Calc\<version> Public documents
	Administrator (user name and password required)	Examples and manuals in /Users/Shared/Thermo-Calc/<version>

OS	User type	Default directory
		To go to this folder, in Finder, from the Go main menu select Go to folder . Enter the above file path and click Go .
	Non root user	home/<user>/Thermo-Calc/<version>
	Root user	usr/local/Thermo-Calc/<version>

2.5.1 Graphical Mode Examples

These project files have the extension *.tcu.

-  Ex_01_Single-point_equilibrium.tcu
-  Ex_02_Step_in_temperature_in_Fe-C.tcu
-  Ex_03_Fe-C_phase_diagram.tcu
-  Ex_04_Fe-Cr-C_ternary_phase_diagram.tcu
-  Ex_05_Fe-C_stable_and_metastable_phase_diagram.tcu
-  Ex_06_Serial_equilibrium_calculators.tcu
-  Ex_07_User_defined_functions.tcu
-  Ex_08_Scheil_and_equilibrium_solidification.tcu
-  Ex_09_Heat_map_of_carbide_driving_force.tcu
-  Ex_10_Phase_Transition.tcu
-  Ex_11_Coarsening_and_Interfacial_energy.tcu
-  Ex_12_Driving_force_and_Interfacial_energy.tcu

Opening a Project File

Navigate to the file location and double-click the *.tcu file to open it. It launches a new session of the software. Or you can select **File** → **Open Project** from an open session of Thermo-Calc.

 Also see the *Thermo-Calc Graphical Mode Examples Guide*.

Graphical Mode Example Projects

#	Example Description
1	Shows the result from a single-point equilibrium calculation in the Fe-C system. It calculates a single-point equilibrium using the Equilibrium Calculator .
2	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 calculates the stepping in temperature in the Fe-C system using the Equilibrium Calculator and plots it with a Plot Renderer and displays the text using a Table Renderer .
3	Shows the stable Fe-C phase diagram (stable meaning that the graphite phase is entered in the calculation). The same diagram is calculated using a Binary Calculator activity and then a System Definer with an Equilibrium Calculator activity.
4	Shows a ternary phase diagram in the Fe-Cr-C system at 1000 K. The same diagram is calculated using a Ternary Calculator and then a System Definer with an Equilibrium Calculator activity.

#	Example Description
5	Shows how to overlay results from two calculations (the stable and the metastable Fe-C phase diagrams) in the same plot using the Equilibrium Calculator .
6	Shows how to use serially coupled Equilibrium Calculators for more complex equilibrium conditions. Four examples using the Equilibrium Calculator help you learn how to do this in Thermo-Calc.
7	Shows the use of user-defined functions. A series of equilibria for an Fe-Cr-C alloy are calculated by varying temperature between 500 and 3000 K using the Equilibrium Calculator .
8	Shows a comparison for an Al-Si alloy solidified under full local equilibrium and under the Scheil assumptions using the Scheil Calculator .
9	Shows how to use <i>property grid</i> calculations to plot the driving force for a carbide as a function of two composition variables. The final plot, using the Plot Renderer , can be either a heat map or a contour plot.
10	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.
11	Uses the Property Model Calculator and both thermodynamic and kinetic demonstration steel databases. With a grid calculation type it produces three plots: a heat map, a contour plot and a cross plot with contour (where both the interfacial energy and coarsening rate is shown).
12	Uses the Property Model Calculator and both thermodynamic and kinetic demonstration steel databases. Using a grid calculation type it produces a contour plot comparing the driving force and interfacial energy.

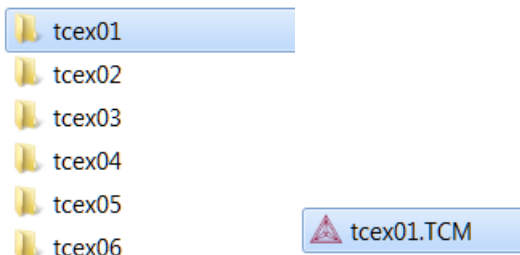
2.5.2 Console Mode Examples

These macro files (with the extension *.TCM) include comments, which you can either run in Thermo-Calc or open and read in a text editor. If you 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. However, the PDF guide, *Thermo-Calc Console Mode Examples Guide* (see [Figure 1](#)), also shows the output for each example.

Opening a Macro File

Navigate to the file location, where each example is in its own folder.

Name




In the folder, double-click the *.TCM file to open it. It launches a new session of Thermo-Calc and opens in Console Mode. If you have an instance of Thermo-Calc open in Console Mode, you can also drag and drop the file to run the macro. You can also open any text file editor and drag the file into it to see its contents.

Console Mode Macro Examples

#	Example Description
1	Calculation of the binary Fe-C phase diagram.
2	Plotting of thermodynamic functions in unary, binary and ternary systems and working with partial derivatives and partial quantities
3	Calculation of an isothermal section using the TERNARY module.
4	Calculation of the miscibility gap in Fe-Cr
5	Calculation of a vertical section from Al to 30% Mg ₂ Si
6	<p>Calculation of an isopleth in low alloyed Fe-Mn-Si-Cr-Ni-C steel.</p> <p>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 command. Hidden commands set the pressure to 1 bar and so that iron is "the rest".</p> <p>After calculating the first equilibrium a phase diagram is calculated with one axis variable as temperature and the other as the carbon content.</p>
7	<p>Calculation of single equilibria in low alloyed Fe-Mn-Si-Cr-Ni-C steel.</p> <p>There are two general ways to perform a single equilibrium calculation:</p> <ul style="list-style-type: none"> • Get data from a database, then in POLY use SET_CONDITION and COMPUTE_EQUILIBRIUM. • Go directly to POLY and use DEFINE_MATERIAL. <p>The COMPUTE_TRANSITION command is also used to determine the temperature or composition where one phase forms or disappears.</p>
8	Calculation of property diagrams for a high speed steel i.e. phase fraction plots, activity vs temperature, etc.
9	Calculation of dew point.

#	Example Description
10	<p>The example calculates an equilibrium with suspended or dormant phases and shows how to avoid clogging of Cr₂O₃ in a continuous casting process. 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.</p> <p>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.</p>
11	<p>This example demonstrates the oxidation of Cu₂S with 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.</p> <p>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 POLY_3. 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.</p>
12	This example shows a number of independent cases using the TAB- module to tabulate thermodynamic data for reactions.
13	Binary calculation of Al-Ti phase diagram and G curve.
14	Calculation of heat and heat capacity variations during solidification of an Al-Mg-Si alloy.
15	<p>Solidification simulation of a Cr-Ni alloy using the SCHEIL module.</p> <p>There is no back diffusion in the solid.</p>
16	Calculation of the second order transition line in the Bcc field of the Al-Fe system.
17	<p>Calculation of pseudo- or quasi-binary phase diagram in the CaO-SiO₂ system.</p> <p>This database can be used both for pseudobinary systems like the one in this case, CaO-SiO₂, or for full ternary systems like Ca-Fe-O.</p>
18	<p>Calculation of the A₃ temperature of a steel and the influence of each alloying element on this temperature.</p> <p>A₃ temperature is the temperature where ferrite starts to form from austenite. You can easily read A₃ from an Fe-C phase diagram. But for complex multicomponent steels, no simple diagram can be used. This example shows how to calculate the A₃ temperature of a steel. Using POLY, it is easy to find out the influence of each alloying element on A₃ temperature. This information is useful if you want to modify the compositions of a steel but keep A₃ unchanged.</p>
19A	Mapping of univariant equilibria with the liquid in Al-Cu-Si. Part A. Step-by-step calculation using POLY.

#	Example Description
19B	Mapping of univariant equilibria with the liquid in Al-Cu-Si. Part B. Using the TERNARY module, you can get the information on invariant reactions, such as temperature and compositions.
20	Calculation of adiabatic decompression in a geological system using the geochemical database.
21	Calculate a ternary isotherm in Fe-Cr-Ni with a user-defined database.
22	Calculation of a heat balance. In this case C ₃ H ₈ is burned in oxygen and the adiabatic flame temperature is calculated.
23	Calculation of a para-equilibrium and the T ₀ temperature in a low alloyed steel.
24	<p>Simulation of the silicon arc furnace using the REACTOR module.</p> <p>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.</p> <p>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 their heat content.</p>
25	<p>Simulation of steel refining.</p> <p>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 in order to keep the temperature constant (it is assumed the furnace is isolated and no heat is lost to the environment). This is a typical steel refining process.</p> <p>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.</p>
26	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 AsGa.
27	CVD calculations
28	Example showing calculation of PRE (Pitting Resistance Equivalence) for a duplex stainless steel.
29	Calculation of speciation of a gas
30A	Scheil solidification simulation for Al-4Mg-2Si-2Cu alloy. Part A. Step-by-step calculation using POLY and the STEP_WITH_OPTION command, EVALUATE option.
30B	Scheil solidification simulation for Al-4Mg-2Si-2Cu alloy. Part B. Simulation performed using SCHEIL module.

#	Example Description
31	Calculations of CVM and comparisons with sublattices of a fictitious A B system. Also shows how to overlay diagrams from two calculations.
32	Calculation of oxide layers on steel. Also shows how to append databases.
33	Benchmark calculation - An isopleth in the Fe-Cr-C system.
34	Calculation of the phase diagram and G curves in the Al-Zn system. An example of using the BINARY module.
35	Calculation of potential diagram
36	<p>Assessment - The use of the PARROT module</p> <p>The example is divided into four parts corresponding to the files in the folder.</p> <ul style="list-style-type: none"> • The problem is presented with "selected" experimental data (see the <i>tcex.36.readme</i> file). 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 (<i>tcex36a.TCM</i>) • The creation of the experimental data file is described (<i>tcex 36b.TCM</i>) • The actual run in the PARROT module in order to obtain the result (<i>tcex 36cpd.TCM</i>)
37	Calculation of an isothermal section using command lines.
38	Calculation of the Morral "rose" (miscibility gaps).
39	<p>This example shows how Thermo-Calc calculates the reversible Carnot cycle of a heat engine using one mole of an ideal gas with two fictitious species A and A₂.</p> <p>The Reversible Carnot cycles are usually drawn schematically. Using Thermo-Calc and realistic data it is possible to calculate a reversible Carnot cycle of a heat engine and to relate it to different thermodynamic quantities.</p> <p>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.</p>
40	<p>A series of examples designed to demonstrate the advanced POURBAIX module calculations and graphical processing. Also see the text file the Extended folder (<i>TCEX40-README.txt</i>).</p> <p>The first example automatically calculates and plots a Pourbaix diagram for 0.001 m Fe in a 0.1 m NaCl aqueous solution at 25C and 1 bar. 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.</p> <p> For details about the other examples, see Pourbaix Examples TCEX40, 40A to 40E, and TCEX53.</p>
41	Calculation of a solubility product. Shows the STEP_WITH_OPTION command, T-ZERO option.

#	Example Description
42	Formation of para-pearlite (isopleth calculation) Fe-Mn-C system at 2.5%Mn Mass u-fraction (an example of a paraequilibrium calculation).
43	Formation of para-pearlite (calculation of isothermal section) Fe-Mn-C system at 700 C (an example of a paraequilibrium calculation).
44	This example uses variables and functions to predict properties e.g. proof strength for an austenitic stainless steel at elevated temperatures (20-550C).
45	3D-diagram that calculates the gamma volume in the Fe-Cr-C system. To view the generated file, <i>tcex45.wrl</i> , install a WRML (Wirtual Reality Modelling Language) viewer to the web browser. WRML viewers can be downloaded from various sites, e.g. www.parallelgraphics.com or www.sim.no .
46	3D-diagram that calculates the liquidus surface of the Fe-Cr-C system. To view the generated file, <i>tcex46_tri.wrl</i> and <i>tcex46_sqrt</i> , install a WRML (Wirtual Reality Modelling Language) viewer to the web browser. WRML viewers can be downloaded from various sites, e.g. www.parallelgraphics.com or www.sim.no .
47	3D-quaternary diagram that calculates the gamma volume in the Fe-Cr-V-C system at 1373K. To view the generated file, <i>tcex47.wrl</i> , install a WRML (Wirtual Reality Modelling Language) viewer to the web browser. WRML viewers can be downloaded from various sites, e.g. www.parallelgraphics.com or www.sim.no .
48	This is an example of Scheil solidification with C back diffusion in solid phases and compares it with simple Scheil and equilibrium calculations.
49	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.
50	This example shows the quasichemical model using TDB to replicate figures 3 and 4 from Kongoli, F., Pelton, A. D. & Dessureault, Y. Thermodynamic modeling of liquid Fe-Ni-Cu-Co-S mattes. <i>Metall. Mater. Trans. B</i> 29, 591–601 (1998).
51	Calculation of molar volume, thermal expansivity and density.
52	This example shows how to change the excess models for binary/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 TDB module. <ul style="list-style-type: none"> • For binary excess model: from the default R-K model to Mixed-Excess-Model (Note the phase has to be a substitutional phase) • For Ternary Extrapolation Model: from the default R-K-M model to Toop_Kohler model.
53	Pourbaix Diagram Calculations through the TDB-GES-POLY-POST routine. Using PAQ2 or PAQS2 database; for the Fe-X-H ₂ O-NaCl heterogeneous interaction systems (X = Cr-Ni-Co).

2.6 The Thermo-Calc Modules and Activities

Although many calculations can be done in either Graphical or Console Mode, only data optimisation and thermodynamic or kinetic assessments are available in Console Mode. Conversely, only the Property Model Calculator is available in Graphical Mode.

Modules and Activities briefly describes 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 activities. Some modules require additional licenses.

The Graphical Mode column indicates whether there is an equivalent activity available in Graphical mode.

 For the Console Mode only commands see [The Console Mode Interface](#) and the *Thermo-Calc Console Mode Command Reference*.

Modules and Activities

Full Module Name in Console Mode	Short Name	Graphical Mode Activity	Primary Functions
BINARY_DIAGRAM_EASY	BIN	Binary Calculator	Calculate binary phase diagrams. Access to specific databases designed for BIN, such as TCBIN, is required.
DATABASE_RETRIEVAL	DATA	System Definer	Select appropriate databases, define chemical systems and retrieve the data required for calculations.
DICTRA_MONITOR ¹	DICTRA	Console Mode only	Run simulations of diffusion controlled transformations in Thermo-Calc.
DIC_PARROT ¹	DIC_PARROT	Console Mode only	This is the data optimisation module for DICTRA. It allows you to assess experimental data and use such data to optimise calculations.
EDIT_EXPERIMENTS	ED_EXP	Console Mode only	Part of the PARROT submodule, use it to edit experimental data points to make reliable optimisations.
GIBBS_ENERGY_SYSTEM	GIBBS	Console Mode only	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.

Full Module Name in Console Mode	Short Name	Graphical Mode Activity	Primary Functions
PARROT	PARROT	Console Mode only	A data optimisation module to assess experimental data and use the data to optimise calculations.
not available	-	Property Model Calculator	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.
POLY-3	POLY	Equilibrium Calculator	Equilibrium calculation module. Specify conditions and make calculations.
POST_PROCESSOR	POST	Plot Renderer	For post-processing and plotting of calculation results. Modify property and phase diagrams, add labels, change the diagram colours, etc. Submodules to POLY-3 and DICTRA for example.
POTENTIAL_DIAGRAM	POTENTIAL	Ternary Calculator	Calculate and plot gas potential diagrams in a ternary system. The potential of two gas species are used as the diagram axes.
POURBAIX_DIAGRAM	POURBAIX	Console Mode only	Calculate and plot pH-Eh diagrams (Pourbaix diagrams) and property diagrams for heterogeneous interaction systems involving aqueous solutions.
REACTOR_SIMULATOR_3	REACTOR	Console Mode only	Simulate chemical reaction processes in several feed-forward steady-state stages or in several dynamic stages.
SCHEIL_SIMULATION	SCHEIL	Scheil Calculator	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).

Full Module Name in Console Mode	Short Name	Graphical Mode Activity	Primary Functions
SYSTEM_UTILITIES	SYS	Console Mode only	In Console Mode, interact with the operating system and change environmental settings. Create and execute MACRO files.
TABULATE_REACTION	TAB	Console Mode only	Tabulate properties of chemical reactions and substances (stoichiometric or solution phases).
TERNARY_DIAGRAM	TERN	Ternary Calculator	Calculate ternary phase diagrams.

2.7 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**.

[Figure 2](#) is an example of the **License Information** window for a network client installation.

 Also see the [Thermo-Calc Installation Guide](#) for more about license types.

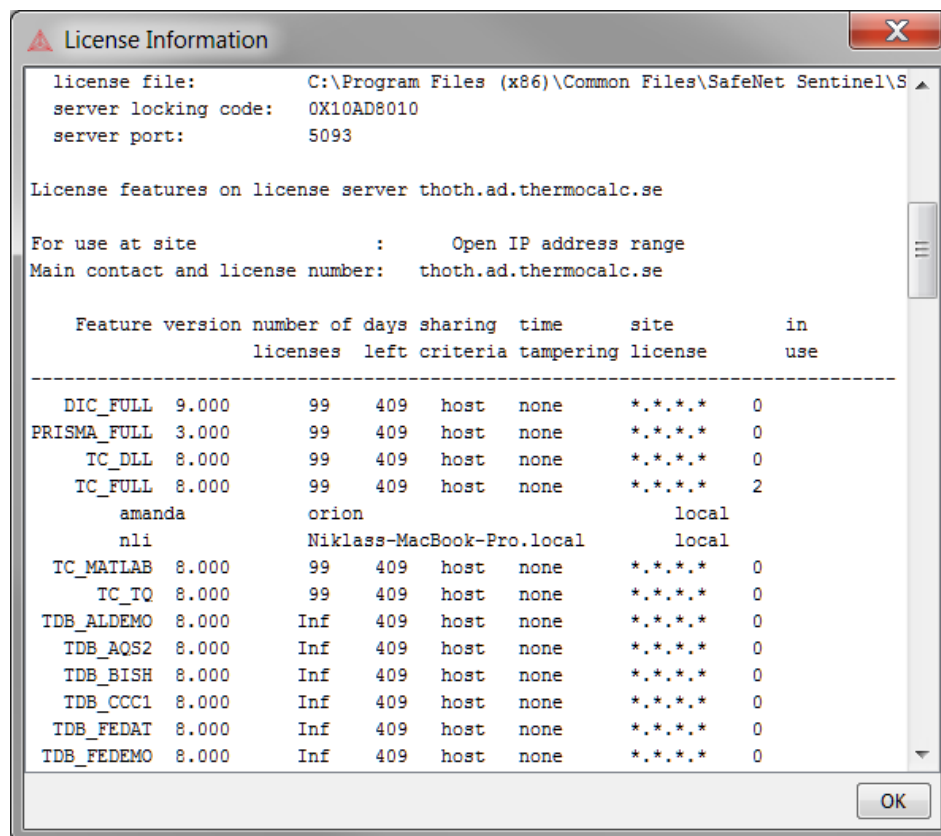


Figure 2: License window for a network installation.

- 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.
- Under each license type with instances checked out, there is a list of who checked out each license. In the example, two users, *amanda* and *nli*, have licenses checked out.
 - 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.
 - 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.
- There is also site and user information available.

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 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 optimisation 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. See [Figure 2](#).

2.8 Databases

Depending on the type of license and operating system, the databases 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** (file path is *C:\Program Files\Thermo-Calc\2015b\data*).



All databases have the file extension **.TCD**.

In Graphical Mode you may need to navigate to a database file location. For example, in the [System Definer](#) activity you can click **Open user database to choose a database**.

2.8.1 Database Checker

The Thermo-Calc software includes a program for checking that the syntax of Thermo-Calc database files is correct. This program is intended for advanced users who develop and manage databases.

To launch the Database Checker application, from the main menu select **Tools** → **Database Checker**.

2.9 Using This Guide

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

This user guide is a supplement to the command references available for Console Mode and DICTRA. Additional documentation and training material is described in [Help Resources](#).

[The Graphical Mode Interface](#) introduces you to the GUI layout and the workflow. In [Graphical Mode Projects](#), it goes into more detail about how to set up and run your projects (with the Quick Start Wizard), using templates, scheduling jobs and creating activities. [The Graphical Mode Activities](#) section specifically describes how to set up each type of available activity in the tree structure.

Console Mode has more functionality than Graphical Mode but the underlying concepts are the same. There are, however, command lines and extensive details applicable to this mode. This guide is only the beginning of the learning objectives. In particular, refer to the *Thermo-Calc Console Mode Command Reference* for details about all the commands available.

In this guide it is a basic introduction to the layout of the Command windows, as described in [The Console Mode Interface](#).

Several sections describe and give an example of the calculation types:

- [Equilibrium Calculations](#)
- [Property Diagrams](#)
- [Phase Diagrams](#)
- [Scheil Simulations](#)
- [T0 Temperature Simulations](#)
- [Paraequilibrium](#)
- [Potential Diagrams](#)
- [Aqueous Solutions](#)
- [Tabulation of Chemical Substances, Phases or Reactions](#)

In [Console Mode Visualisation](#) there is an overview of plotting and for both Graphical and Console mode, the [Changing Global Settings](#) section gives information about adjusting global user settings.

3. The Graphical Mode Interface

This section introduces you to the concepts and terminology of Graphical Mode and describes the basic workflow.

👁 Also see [The Console Mode Interface](#).

- [The GUI Layout](#)
- [Project Activities and the Tree Structure](#)
- [Activity Successor and Predecessor Nodes](#)
- [Graphical Mode Workflow](#)
- [Main Menu and Toolbar](#)
- [Saving and Opening Thermo-Calc Project Files](#)
- [Project Activity Nodes](#)
- [Project and Activity Menus](#)
- [Moving Windows](#)
- [Moving Nodes in the Tree and Using the Grid](#)
- [Node Status Markers](#)

3.1 The GUI Layout

[Figure 3](#) is an example of the default GUI layout for Graphical Mode. You can easily reorganize these windows.

👁 Also see [Moving Windows](#).

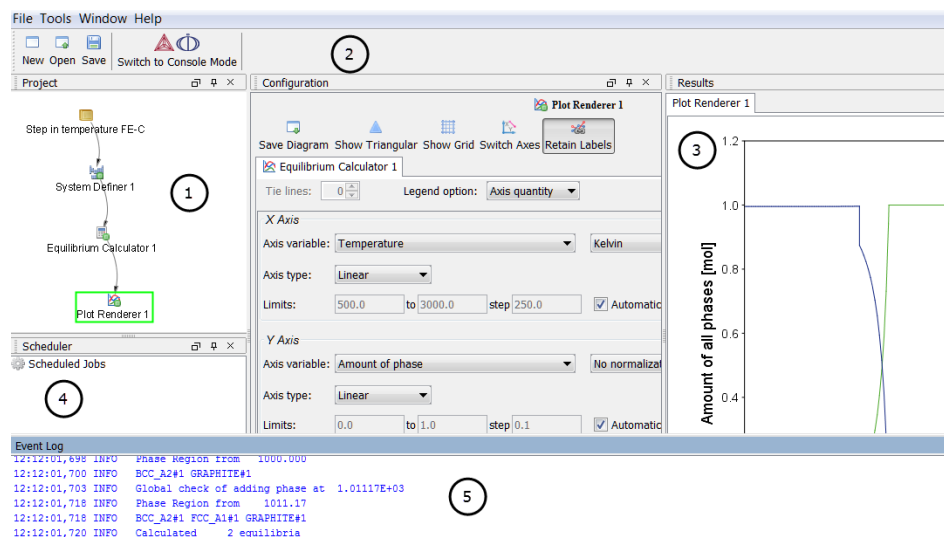


Figure 3: The Graphical Mode default window layout. Note that the Results window also has a Plot Renderer tab in this example. You can also have a Table Renderer tab.

The windows in [Figure 3](#) are:

1. **Project:** Create, manipulate and navigate between the activities that make up a project.
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.

3.2 Project Activities and the Tree Structure

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 (see [Activity Successor and Predecessor Nodes](#) for definitions). When working with activities in the Project window these are also referred to as *nodes* (or *activity nodes*) in the tree structure.

The Project window in [Figure 4](#) shows a My Project node with two trees. In each tree, settings and calculation results are propagated downward until the calculation and the visualisation 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.

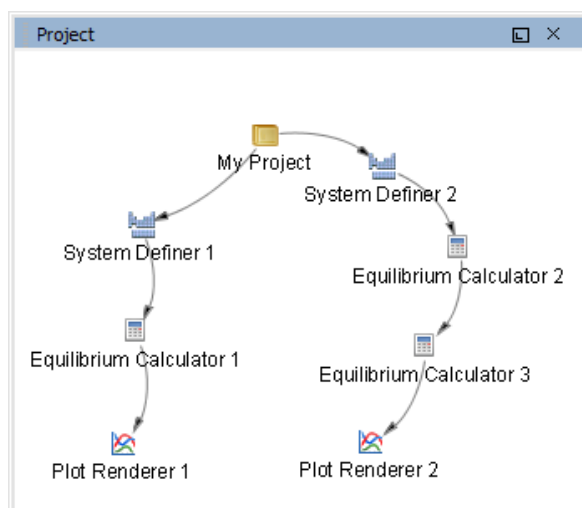


Figure 4: An example of a project with two trees with successor and predecessor activity nodes.

3.3 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.

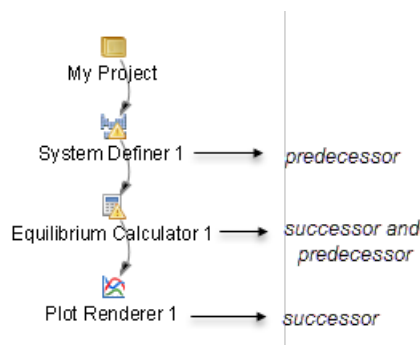


Figure 5: Predecessor and successor nodes in the tree structure.

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.

[Figure 6](#) is an example of a Project window with successors and predecessors. For example, **Binary Calculator 1** is a predecessor to the successors, **Plot Renderer 2** and **Table Renderer 1**.

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

 Also see [Project and Activity Menus](#).

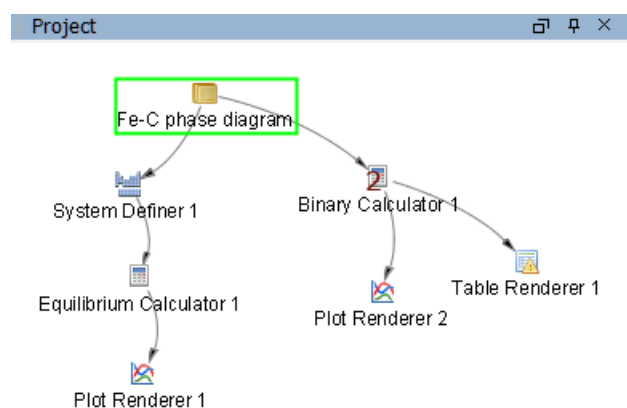


Figure 6: An example of successors and predecessors.

3.3.1 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.

 Also see [Cloning Activities and Trees](#).

Predecessors and Successors by Activity

Activity	Possible predecessors	Possible successors
My Project	None; this is the first node of the tree structure	System Definer, Binary Calculator, Ternary Calculator, Experimental File Reader. Also choose templates from this level.
System Definer	My Project, System Definer	Property Model Calculator, Equilibrium Calculator, Scheil Calculator
Property Model Calculator	System Definer	Plot Renderer
Equilibrium Calculator	System Definer, Equilibrium Calculator	Equilibrium Calculator, Plot Renderer, Table Renderer
Plot Renderer	Property Model Calculator, Equilibrium Calculator, Binary Calculator, Ternary Calculator, Scheil Calculator, Experimental File Reader	None
Table Renderer	Equilibrium Calculator, Binary Calculator, Scheil Calculator	None
Experimental File Reader	My Project	Plot Renderer
Binary Calculator	My Project	Plot Renderer, Table Renderer
Ternary Calculator	My Project	Plot Renderer
Scheil Calculator	System Definer	Plot Renderer, Table Renderer

3.4 Graphical Mode 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.

The typical workflow is to:

1. *Define a system:* Create a [System Definer](#) activity (in the **Project** window) where you select a database and the elements to have as system components (in the **Configuration** window).

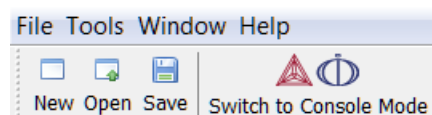
2. *Set up and run a calculation:* Create an [Equilibrium Calculator](#) activity (a successor to the **System Definer**), where calculation conditions are set (temperature, pressure, etc.). This is where axis variables are set to create a property or phase diagram. These settings are also made in the **Configuration** window. You can also create a [Property Model Calculator](#).
3. *Visualize the results:* Create either a [Plot Renderer](#) or a [Table Renderer](#) 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.

3.5 Main Menu and Toolbar

Along the top of the GUI is a toolbar and menus as described in this section.



Graphical Mode Menu and Toolbar Options lists the main menu and toolbar options. 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 instead. These are discussed in [The Console Mode Interface](#) section.

Graphical Mode Menu and Toolbar Options

Option	Description	Action (s)
New	Create a new project.	Click New on the toolbar. Select File → New Project . Press <Ctrl+N>.
Open	Open an existing project. See Saving and Opening Thermo-Calc Project Files .	Click Open on the toolbar. Select File → Open Project . Press <Ctrl+O>.
Save	Save a project. See Saving and Opening Thermo-Calc Project Files .	Click Save on the toolbar. Select File → Save Project . Press <Ctrl+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.
Append Project	Combine two projects into one project file. See Saving and Opening Thermo-Calc Project Files .	Select File → Append Project .

Option	Description	Action (s)
Save Project As...	Save an existing project with a new name.	Select File → Save Project As...
Exit	Exit the program.	In the upper right-corner of the program, click the X. Select File → Exit . Press <Ctrl+Q>.
Options	Change the global defaults for a variety of settings. See Changing Global Settings .	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.
Online Help	Open the online help system where you can browse or search all the Thermo-Calc documentation.	Select Help → Online Help
Show License Info	Open the License Information window. See Displaying Thermo-Calc License Information and the <i>Thermo-Calc Installation Guide</i> for more information.	Select Help → Show License Info
Check for update	Check the Thermo-Calc Software website for updates to the software.	Select Help → Check for update

3.6 Saving and Opening Thermo-Calc Project Files

Thermo-Calc Graphical Mode uses project files with the file name suffix **.TCU**.

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.

To open a Thermo-Calc project file, on the toolbar click **Open** and select the project file in the **Open file** window.



You can only have one project file open at a time. 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.

 Also see [Saving Plots](#) and [Saving Tabulated Data](#).

3.7 Project Activity Nodes

Project Activity Node Descriptions is a brief description of the project activity types. When working with activities in the Project window these are also referred to as nodes.

Project Activity Node Descriptions

Activity type	Description
System Definer	Define a certain thermodynamic system and read it from file into memory.
Property Model Calculator	Choose one or more general 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	Set thermodynamic conditions and define axis variables when a series of equilibrium calculations are to be performed in one or more dimensions.
Plot Renderer	Determine the layout of non-text based output.
Table Renderer	Use it for text-based output.
Binary Calculator	<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> <p> To perform this activity, you need a database designed for the Binary Calculator, such as the TCBIN database.</p>
Ternary Calculator	<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> <p> To get a reliable result you need a database that fully assesses binary and ternary systems.</p>
Scheil Calculator	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.
Experimental File Reader	Read experimental data files (*.EXP). This type of file contains information specifying a plotted diagram, written in the DATAPLOT graphical language. For more information about DATAPLOT, search the online help or refer to the <i>DATAPLOT User Guide</i> .

3.8 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 menu shown in [Figure 7](#). Most nodes in the tree have a common menu as shown in [Figure 8](#), with differences due to placement in the tree and the activity type.

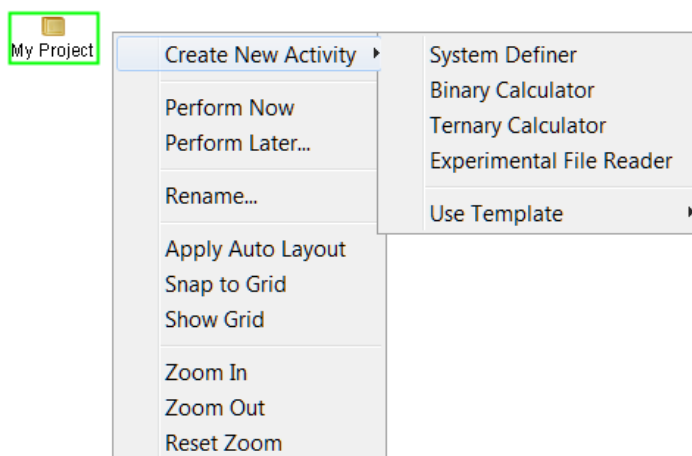


Figure 7: Menu options available for the My Project node.

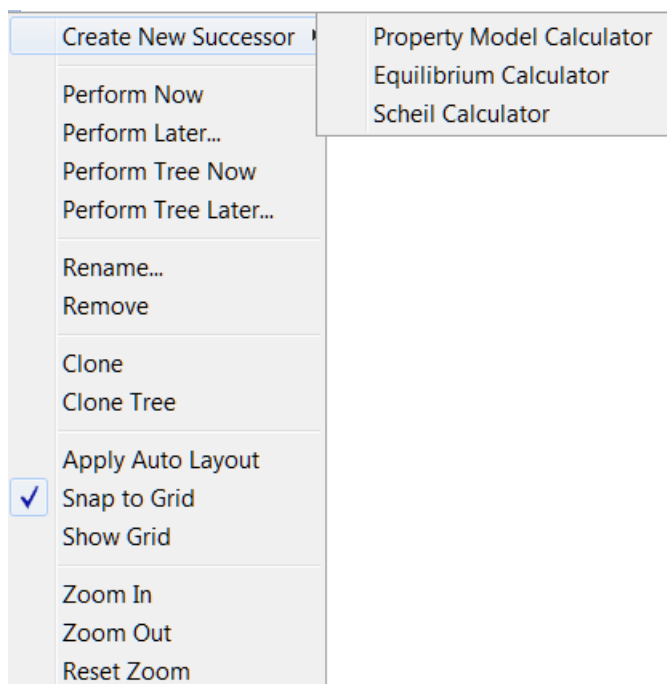


Figure 8: An example of the common menu for other activities.

Menu Options for Activities

Option	Description	Action (s)
Create New Activity	Add System Definer, Binary Calculator, Ternary Calculator, and Experimental File Reader nodes.	Right-click My Project and from the Create New Activity menu choose an option.

Option	Description	Action (s)
	See Creating Activities and Successors .	
Create New Activity → Use Template	Choose from the available templates to use the Wizard or add predefined nodes. See Creating a Project from a Template .	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.
Create New Successor	Add a successor to the selected node. Options are System Definer, Equilibrium Calculator or Scheil Calculator. See Creating Activities and Successors .	Right-click one of these nodes System Definer, Property Model Calculator, Equilibrium Calculator, Binary Calculator, Ternary Calculator or Experimental File Reader , and from the Create New Successor menu choose an option.
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. See Using the Scheduler .	Right-click any node.
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. See Cloning Activities and Trees .	Right-click any node except My Project.
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. See Moving Nodes in the Tree and Using the Grid .	Right-click any node.
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.

3.9 Moving Windows







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

By default, the windows are fixed and open, except the **Event Log** window, which is set to auto-hide by default.

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

Floating, Hiding and Minimizing Windows in the GUI

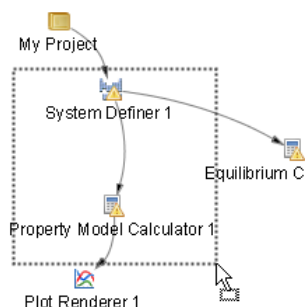
For each window you can rearrange, resize, minimize and close it. At the top right corner are the buttons listed in the table.

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

3.10 Moving Nodes in the Tree and Using the Grid

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

- Click an activity node to *select* it.
- To select several activities, hold down <Ctrl> while clicking on the nodes 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.



- To move activities, click and hold the activity node and move the cursor.
- Zoom in and out with the mouse scroll wheel.

- In the **Project** window right-click and select **Zoom In** or **Zoom Out**. To go back to the default zoom, select **Reset Zoom**.
- To show a grid of light-grey cross-hairs overlaid on a project (see [Figure 9](#)), 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.

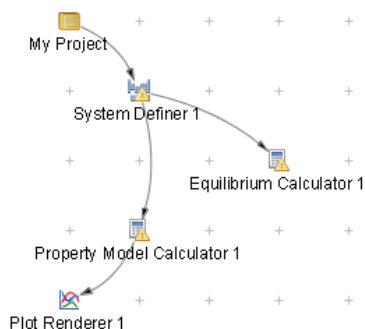










Figure 9: The project window with the grid turned on and activity nodes moved from the default location. These nodes are snapped to the grid.

3.11 Node 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 icons in the **Project** window. The status markers are displayed on a System Definer icon.

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.
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.

4. Graphical Mode Projects

This section describes how you create, perform and link activities.

- [The Quick Start Wizard](#)
- [Creating a Project from a Template](#)
- [Cloning Activities and Trees](#)
- [Performing Projects, Trees and Activities](#)
- [Using the Scheduler](#)
- [The Event Log](#)

4.1 The Quick Start Wizard

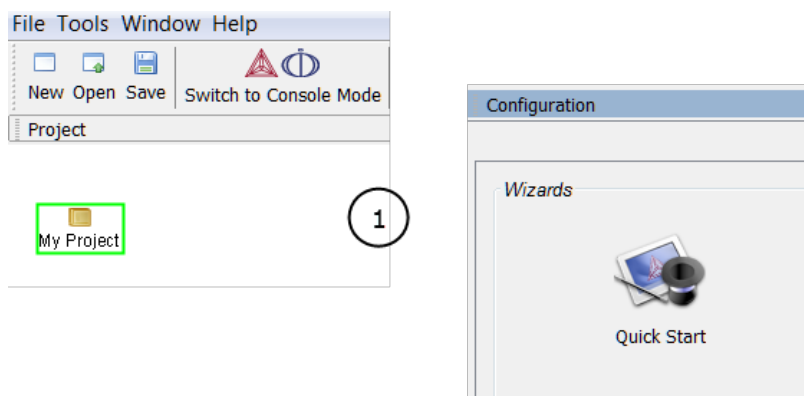
Even before you understand how to work with Thermo-Calc projects, the Quick Start wizard helps you set up a project and run calculations in Graphical Mode. You can set up, calculate and visualize any of the following:

- Single point equilibrium
- Property diagram
- Phase diagram
- Scheil solidification simulation

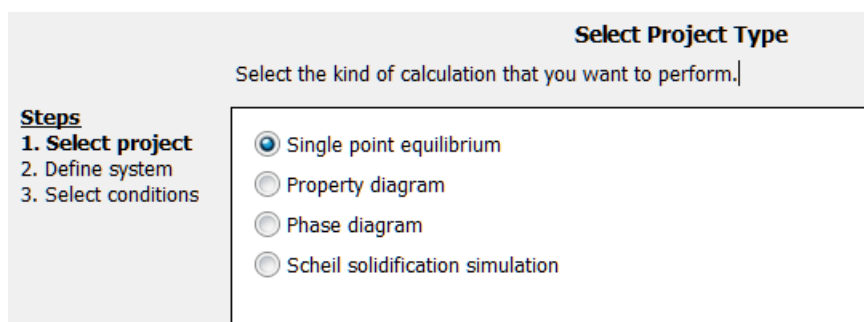
4.1.1 Creating a Project with the Quick Start Wizard

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

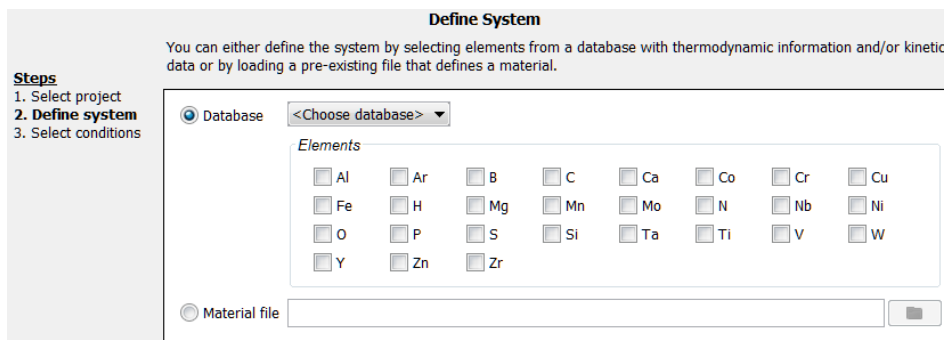
1. In the **Configuration** window click **Quick Start**. If you cannot see the **Quick Start** button, first click **My Project** in the **Project** window.



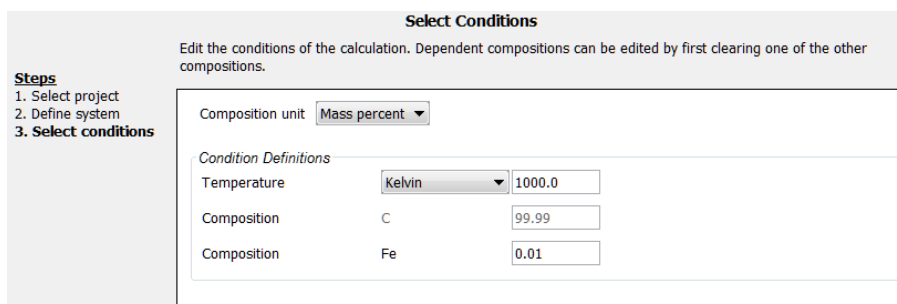
2. In the **Select Project Type** window click to select the type of calculation to perform. **Single point equilibrium**, **Property diagram**, **Phase diagram** or **Scheil solidification simulation**. Click **Next**.



- In the **Define System** window, choose an available **Database**.



- 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.
- 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 **Property diagram** 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.
- Click **Finish**.
 - 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
  
```

9. 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

10. 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**.

4.2 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 as in [Figure 10](#).

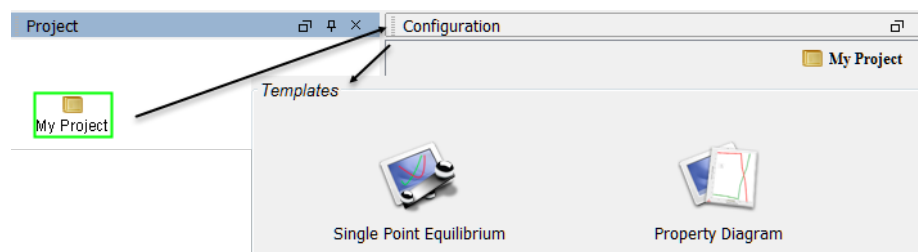
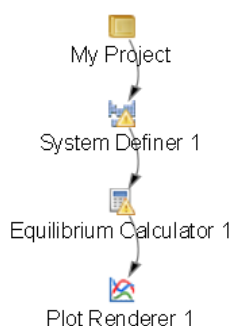


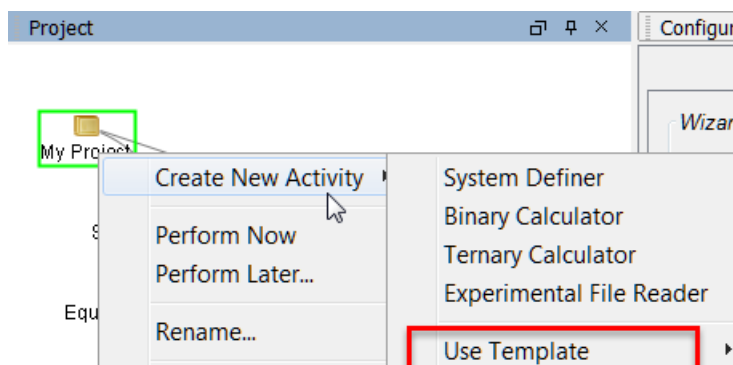
Figure 10: The templates section in the Configuration window.

When you click a template, an activity tree is added to the Project window. You can then configure and perform the activities of the project.

For example, if you click **Property Diagram**, a tree is added to the **My Project** node with **System Definer**, **Equilibrium Calculator** and **Plot Renderer** nodes.



You can also select templates from the Project window. Right-click the **My Project** node and choose templates from the **Create New Activity** → **Use Template** submenu.



4.3 Cloning Activities and Trees

As discussed in [Creating Activities and Successors](#), 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**:

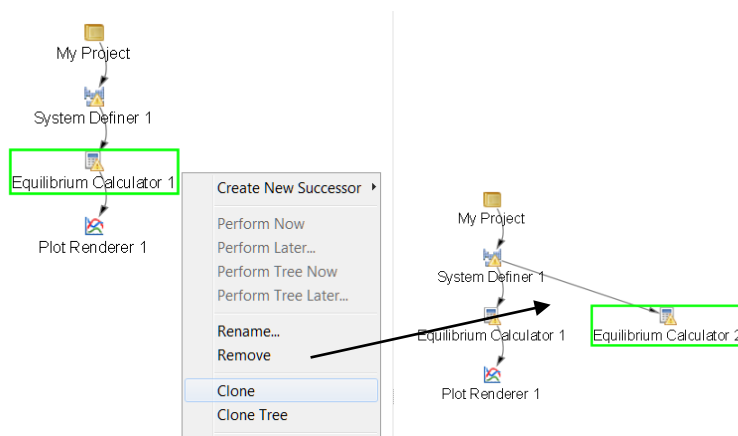



Figure 11: Cloning an Equilibrium Calculator activity node.

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.

4.3.1 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.

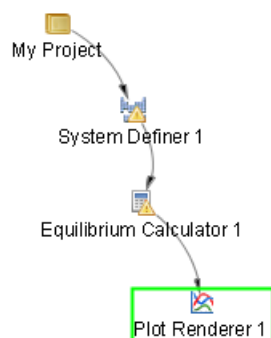
The calculated result from an Equilibrium Calculator that is the predecessor to another Equilibrium Calculator is the starting value for the latter's calculation. The clone of an Equilibrium Calculator on the other hand, does not receive any data as input from the Equilibrium Calculator that it is cloned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

4.4 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).

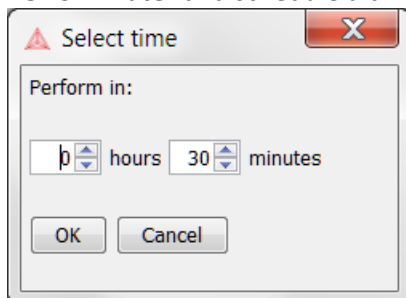
In the **Configuration** window, click **Perform Tree** to perform the currently selected activity and all the activities below it. If there are no activities below the selected activity, then the button says **Perform** instead.

 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 Status Markers](#).

4.5 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.

The following applies to 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.



Also see [Node Status Markers](#).

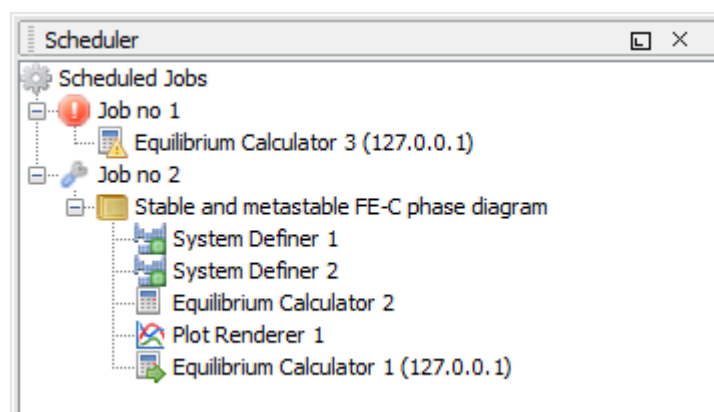


Figure 12: An example of a list of scheduled jobs.

4.5.1 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**.

4.6 The Event Log

The **Event Log** window is closed by default. Click the **Event Log** window once to expand it or select it from the **Window** → **Event Log** menu. Double-clicking the window maximizes the window.

Information about what Thermo-Calc is processing or doing is in blue text and error or warning messages are in red text.

To specify the level of detail in the Event Log window, 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).

 Also see [Changing Global Settings](#).

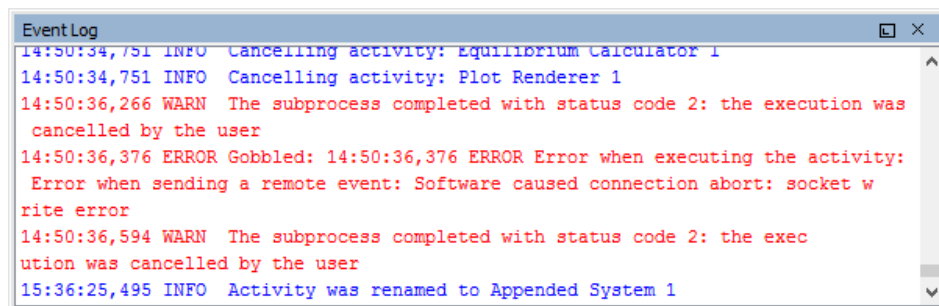


Figure 13: An example of an Event Log with information, warnings and errors.

5. Graphical Mode Activities

This section describes the activity types and has instructions for procedures tied to specific activities.

- [System Definer](#)
- [Property Model Calculator](#)
- [Equilibrium Calculator](#)
- [Plot Renderer](#)
- [Table Renderer](#)
- [Experimental File Reader](#)
- [Binary Calculator](#)
- [Ternary Calculator](#)
- [Scheil Calculator](#)

5.1 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 which species to include as well as change the reference temperature and pressure for your components.

Also see [Creating Activities and Successors](#) for a list of possible successors and predecessors for this activity.

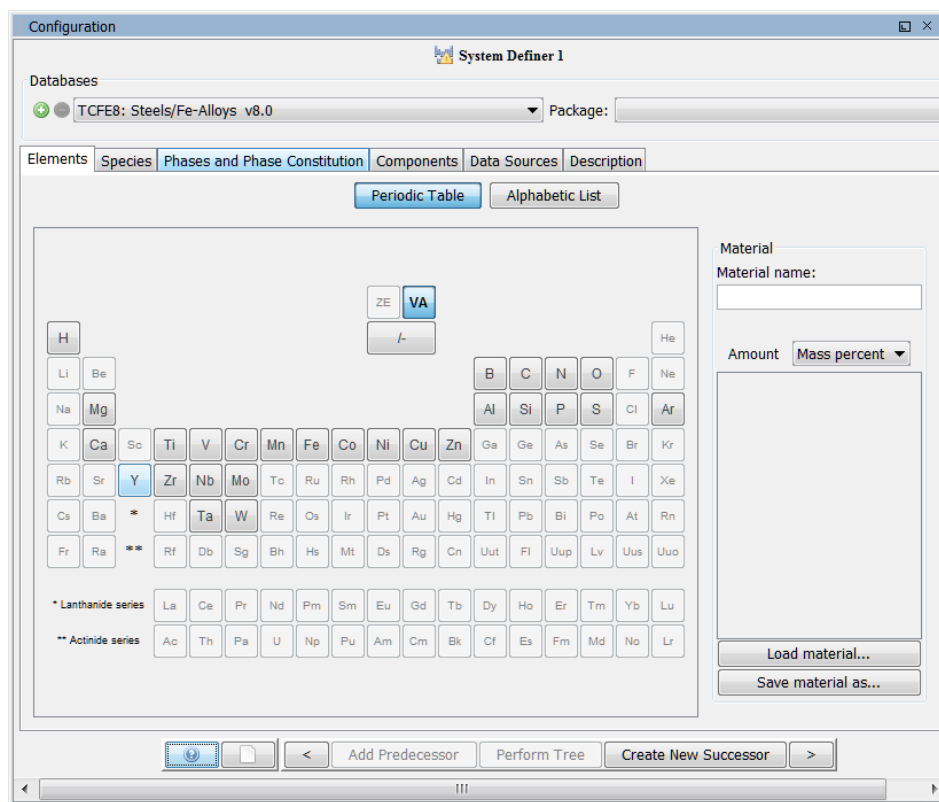
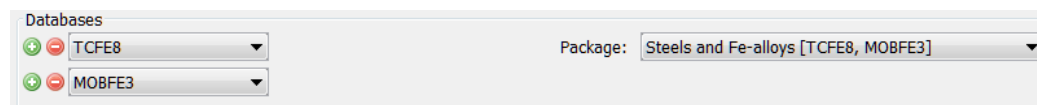



Figure 14: An example of a System Definer Configuration window with a TCFE8 database selected by default.


5.1.1 The System Definer Settings

Choose Database(s) or a Database Package



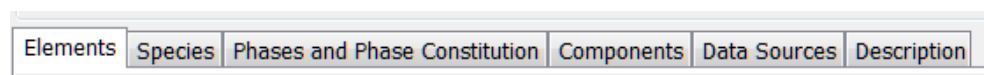
At the top of the **Configuration** window you can choose to add one or more databases by clicking the **Add a database**  button. You can also choose a predefined or custom database package from the **Package** list. Depending on your license, there are predefined database packages available to select.

You can also click **Remove this database**  button as required.

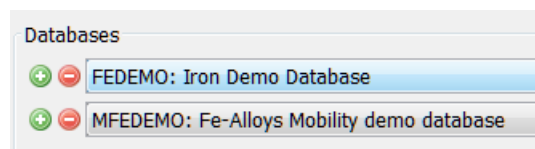
 If you have chosen a database and then remove or change a database, a message displays *Selected databases and selected package may differ*. This means that the original package you selected, which added preset databases, does not match the databases you are using for the project.

 Also see [Clearing a Database Package Message](#).

There are several settings tabs available for the System Definer activity.



The following example uses the FEDEMO and MFEDEMO databases and Example 12 available with the [Graphical Mode Examples](#).



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.

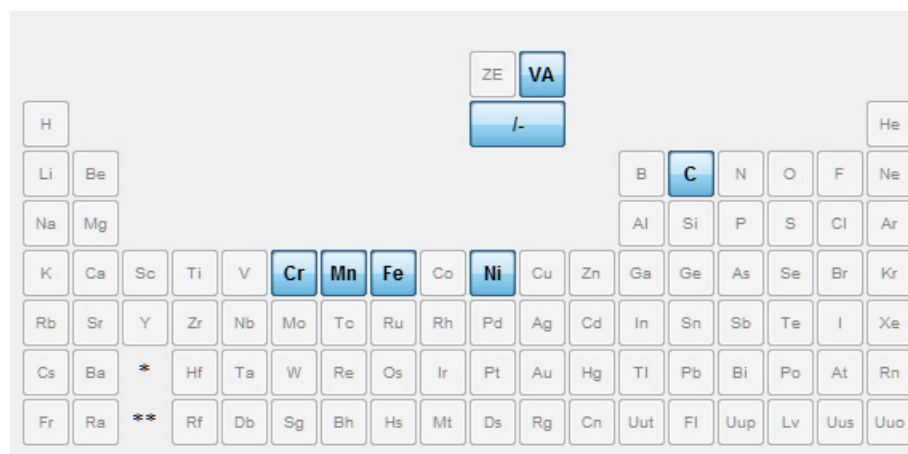


Figure 15: Periodic Table view with available elements for both selected databases. In this example, using the demonstration databases FEDEMO and MFEDEMO, there are only a select number of elements to choose from.

Element	FEDEMO	MFEDEMO
/-	<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"/>

Figure 16: Alphabetic List view with the available elements listed.

On the **Periodic Table** page, you can also define the material composition:

Material
Material name:

Amount

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. Click **Save material as** to save the material you defined, for example **Ferritic**.



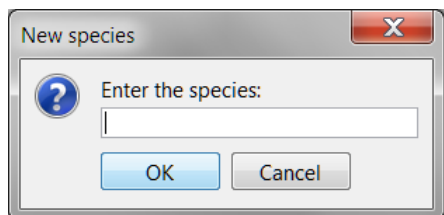
If you Load a material file and then change the composition, a message displays *The composition has changed*. This means that the original values/composition does not match the values you are using for the project. The message is cleared by either reloading the material file or editing the composition field to the original value.

Species

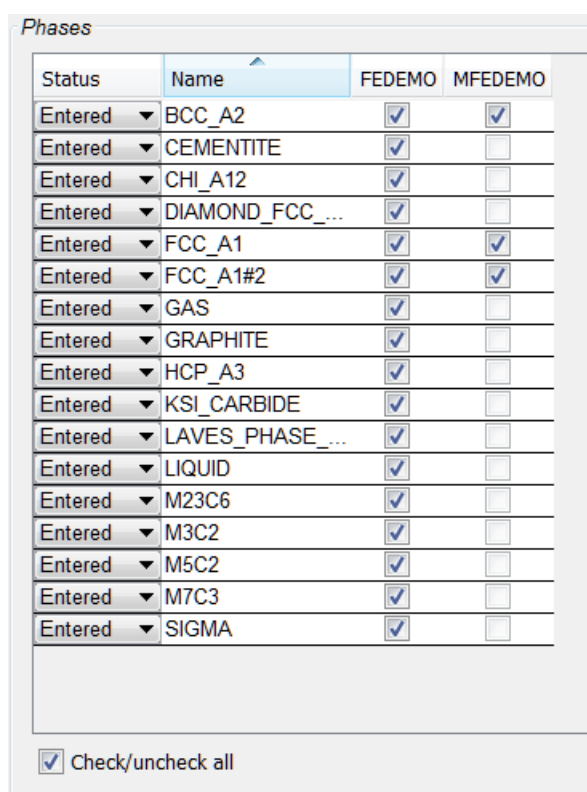
On the **Species** tab for each database you can select and edit the **Species**.

Elements	Species	Phases and Phase Constitution	
Species	Stoichiometry	FEDEMO	MFEDEMO
/-	-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.

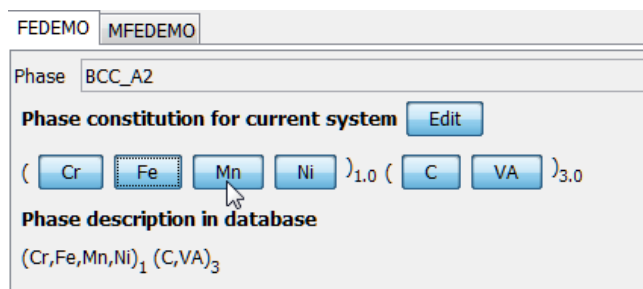


Phases and Phase Constitution



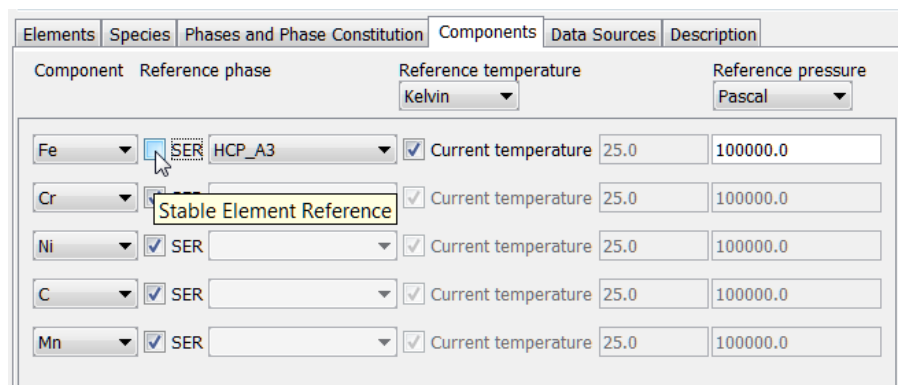
At the top of the **Phases and Phase Constitution** tab for each database, you can review and edit the **Status (Entered or Dormant)** for the selected **Phases**. Select the **Check/uncheck all** check box to toggle between the options.

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.



Components

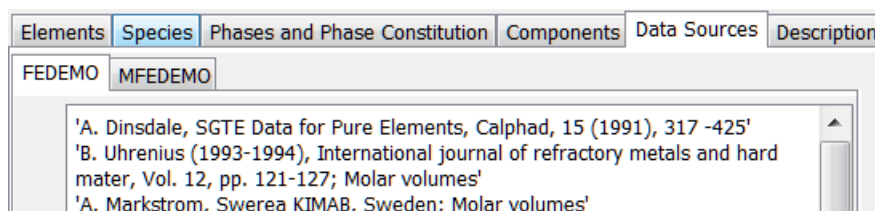
The **Components** tab is where you can review and edit the **Component**, **Reference phase**, **Reference temperature**, and **Reference pressure**. Click to toggle the **SER** (Stable Element Reference) check box on and off. Then choose a **Reference phase** from the list and edit accordingly.



Component	Reference phase	Reference temperature	Reference pressure
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

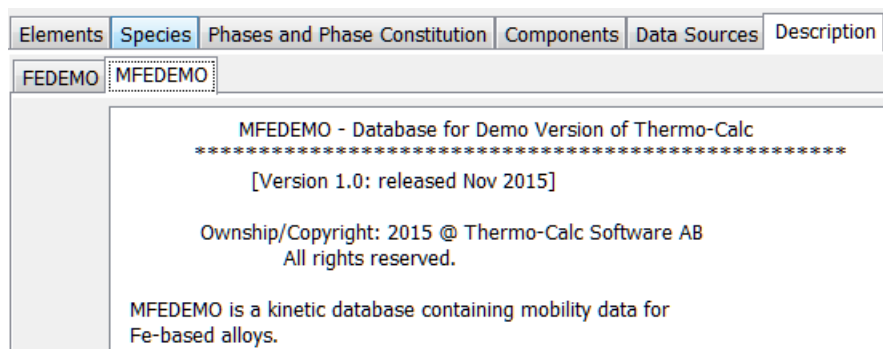
Data Sources

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**.





5.1.2 Creating a System Definer Activity

This section describes how to define a system; specifically how to select one or more databases and define the elements in the system.


 Also see [Databases](#).

1. Right-click **My Project** and from the menu select **Create New Activity** → **System Definer**.
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](#). Options are to:
 - 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.

 To change the default database or create a database package, see [System Definition \(System Definer\)](#) and [Creating a Database Package](#).

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 as indicated and based on the database.

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.

5.2 Property Model Calculator

A Property Model Calculator allows you to predict and optimize material properties. A set of general models is available to use: a [Phase Transition Model](#), [Driving Force Model](#), [Interfacial Energy Model](#), [Coarsening Model](#), and an [Equilibrium Model](#).

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. The **Configuration** window for a Property Model Calculator using the *Phase transition* model is shown in [Figure 17](#) and described in [Defining the Property Model Calculator](#).

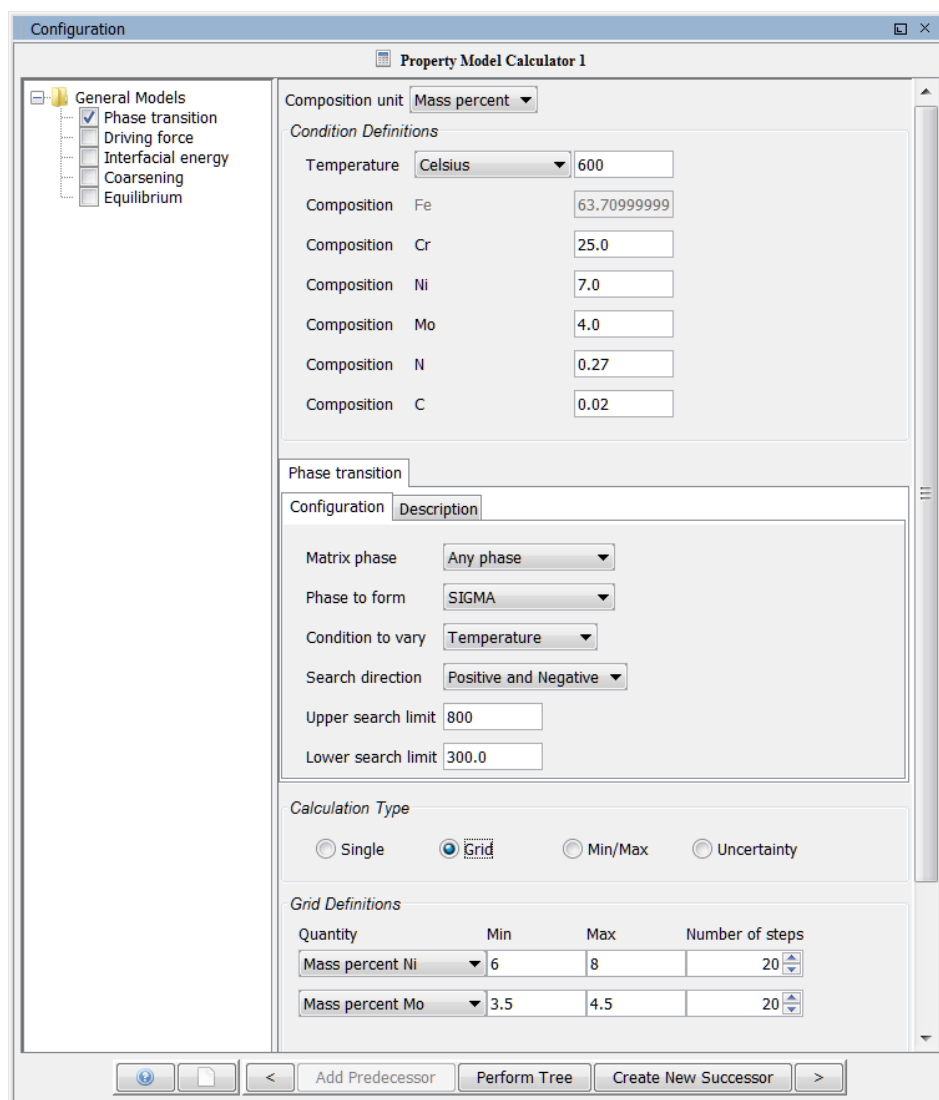


Figure 17: An example of a Property Model Calculator Configuration window.


5.2.1 Property Model Calculator Workflow


When a project is first being designed, it is recommended you test it by first 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 indicating the calculation did not work correctly.

 Also see [Defining the Property Model Calculator](#).

Once the Single calculation type 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.

In general, the workflow for the different models will differ. A recommended start point is to do a Property Diagram calculation to determine what phases you get and where the transitions are before setting up the Property Model Calculator. You can create a Property Diagram using the Quick Start wizard or a template.

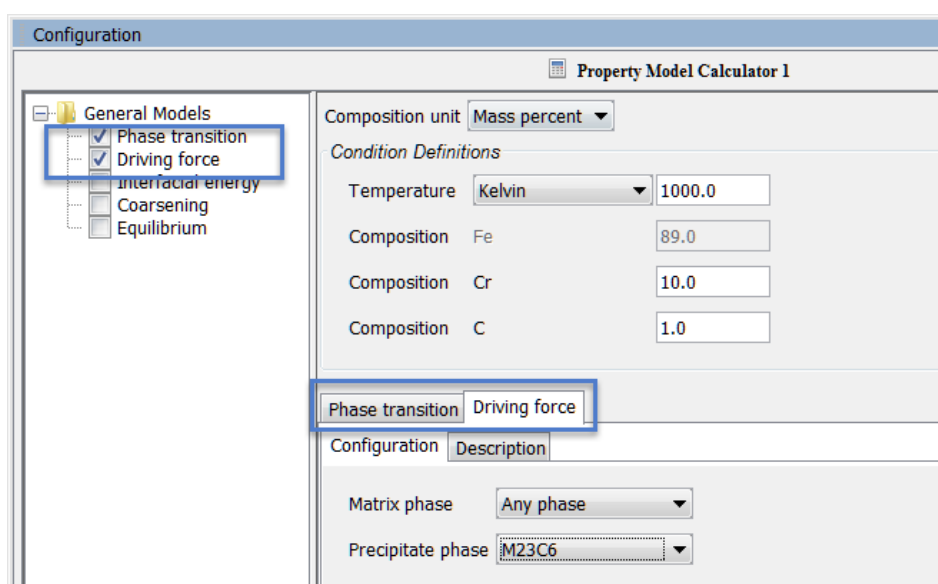
 Also see [The Quick Start Wizard](#) and [Creating a Project from a Template](#).

 For examples using the Property Model Calculator, see examples 10, 11, and 12 in [Graphical Mode Examples](#).

5.2.2 Defining the Property Model Calculator

1. From the left side of the Configuration window, click to select one or more of the check boxes under the **General Models** folder.

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.






2. Enter the settings described in the following table for the *Condition Definitions* and for each *Calculation Type* (Single, Grid, Min/Max, and Uncertainty). For each model on the **Configuration** tab, select or enter settings as required. Click the **Description** tab for more information about the model and refer to the individual sections for more details:

- [Phase Transition Model](#)
- [Driving Force Model](#)
- [Interfacial Energy Model](#)
- [Coarsening Model](#)
- [Equilibrium Model](#)

Property Model Calculator Configuration Settings

Setting/Button	Description
Composition unit	Choose a unit: Mass percent , Mole percent , Mass fraction or Mole fraction
<i>Condition Definitions</i>	Choose a unit (Kelvin , Celsius or Fahrenheit) and then enter a value for the Temperature and Composition .

Setting/Button	Description
	 The values entered in Condition Definitions are used as the start values for the different calculation types.
<i>Calculation Type</i>	<p>Choose a calculation type: Single (no axes), Grid, Min/Max or Uncertainty.</p> <p>For the Single calculation type no further settings are required. The results from this calculation are displayed in the Event Log.</p> <p>Select a Grid to evaluate two axis variables of the selected quantities in the specified range and number of steps.</p> <p>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.</p> <p>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.</p>
<i>Grid Definitions</i>	<p>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.</p>
<i>Min/Max Definitions</i>	<p>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.</p> <p>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.</p>
<i>Sampling of Data from Gaussian Distributions</i>	<p>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. ΔMin/Max is the 95% confidence interval.</p> <p> Also see About the Uncertainty Calculations.</p>
<i>Sampling Parameters</i>	<p>For the Uncertainty calculation type, choose a number of Standard deviations where you want to Truncate the distribution. Choose the Total number of samples.</p> <p> Also see About the Uncertainty Calculations.</p>

About the Uncertainty Calculations

The following example uses the [Phase Transition Model](#) and an **Uncertainty Calculation Type** to describe how the sampling of data is performed. The example (which is example 10 in [Graphical Mode Examples](#)) 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.

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.

An example of a Gaussian distribution is shown in [Figure 18](#). The *mean* is at the peak of the curve (labelled 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.

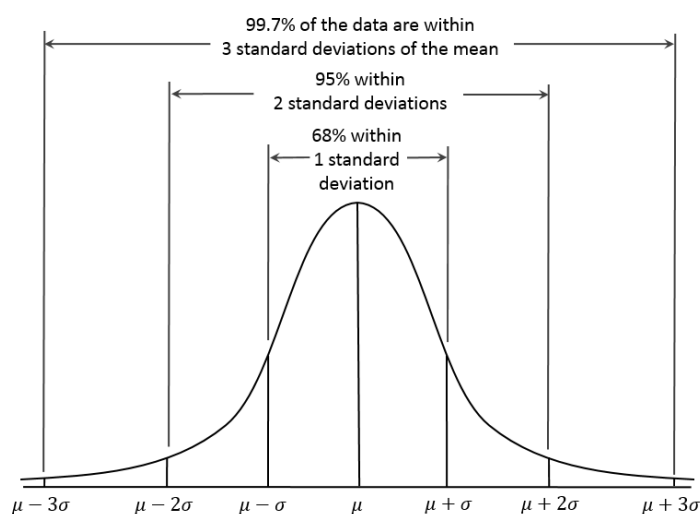
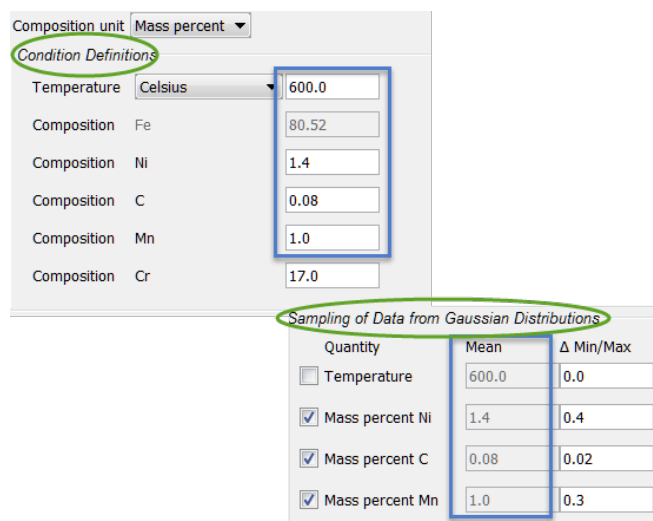


Figure 18: Gaussian distribution, the 3-sigma rule (image by Dan Kernler, https://en.wikipedia.org/wiki/Normal_distribution#/media/File:Empirical_Rule.PNG).

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.

Creating a Histogram Plot

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 ([Figure 19](#)) as the starting point for how much you want to deviate from this value.



Composition unit: Mass percent

Condition Definitions

Quantity	Mean	Δ Min/Max
Temperature	600.0	0.0
Composition Fe	80.52	
Composition Ni	1.4	0.4
Composition C	0.08	0.02
Composition Mn	1.0	0.3
Composition Cr	17.0	

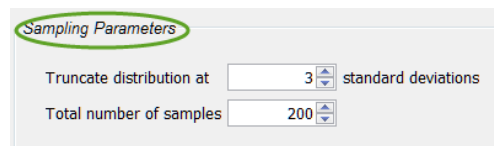
Sampling of Data from Gaussian Distributions

Quantity	Mean	Δ Min/Max
<input type="checkbox"/> Temperature	600.0	0.0
<input checked="" type="checkbox"/> Mass percent Ni	1.4	0.4
<input checked="" type="checkbox"/> Mass percent C	0.08	0.02
<input checked="" type="checkbox"/> Mass percent Mn	1.0	0.3

Figure 19: The mean defined in Condition Definitions is used during the sampling.

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 [Figure 18](#). This confidence interval means that approximately 95% of the sampled values will fall within these limits.

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: 3 standard deviations

Total number of samples: 200

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. For example, on the **Plot Renderer** the variable is set to measure the **Composition** of **Ni**. The initial sample size uses the default, 200, and then, as in [Figure 20](#), the sample size is increased to 300, 400, 600, 800, and 1000 to show how the plot follows the Gauss distribution.

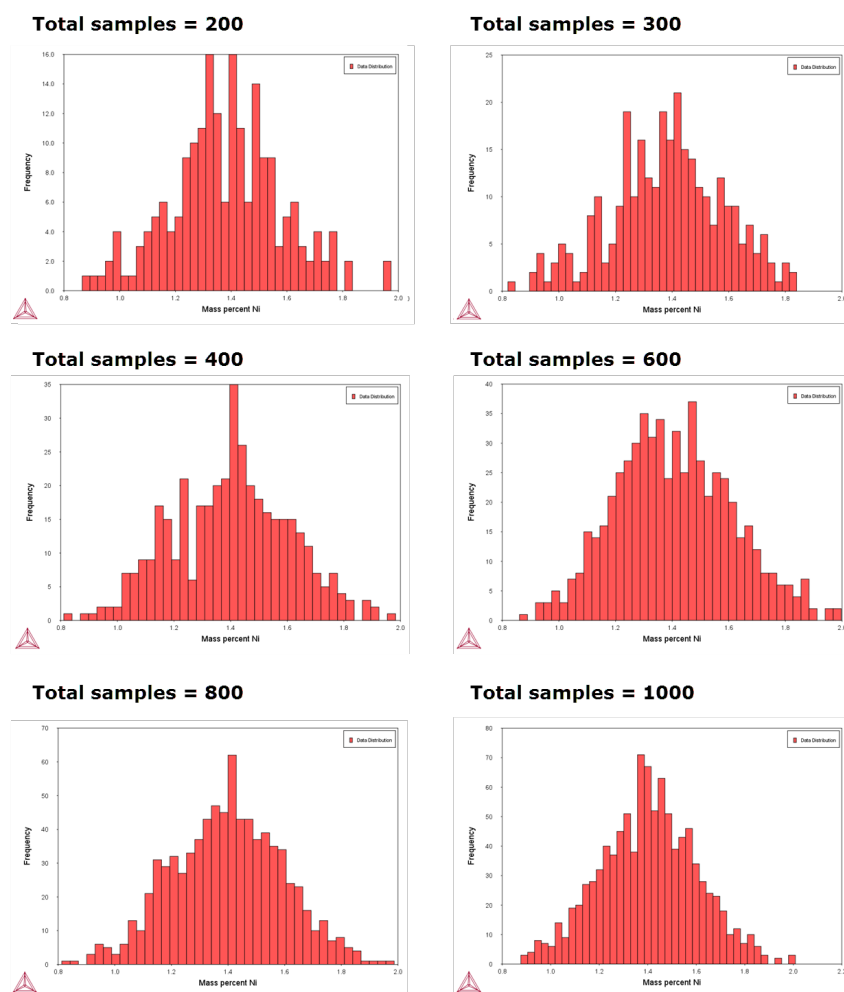


Figure 20: An example of the uncertainty calculations sampling data from Gaussian distributions. This is a series of histogram plots comparing the Ni composition where the total sample size is increased to show how the model follows the Gauss distribution.

Normal Probability Plot

You can also plot the results as a *Normal probability* as shown in [Figure 21](#).

The normal probability plot is a technique used to graphically assess whether a data set is close to being normally distributed. The data set is compared to a theoretical normal distribution and then both results are plotted in the same graph. As long as the points approximately form a straight line, the data set is considered to be normally distributed.

Continuing with this example, on the **Property Model Calculator Configuration** window the X-Axis variable is plotted as **Mass percent Ni** and the Y-Axis variable is plotted as the **Normal probability**.

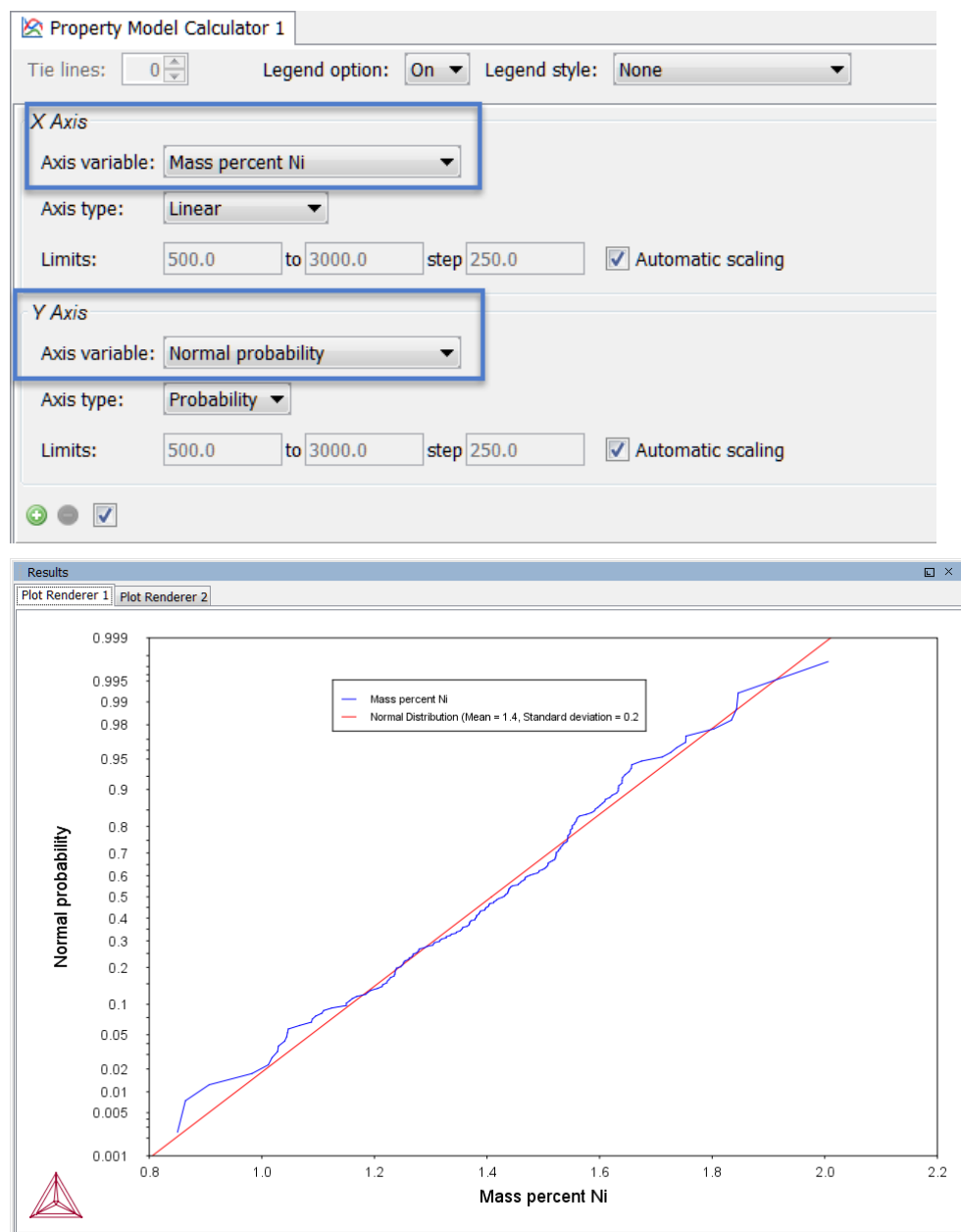


Figure 21: An example of the uncertainty calculations sampling data from Gaussian distributions. This is a normal probability plot comparing the Ni composition where the total sample size is 200. The sampled data (blue line) closely follows the ideal normal distribution (red line). Deviations are naturally 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.

5.2.3 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. 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.
- **Upper search limit** and **Lower search limit** - These values also relate to the search direction, where an estimated change to the released condition implies where a new phase is expected.

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.



For an example of a phase transition model, see example 10 in [Graphical Mode Examples](#).

5.2.4 Driving Force Model

The **Driving Force** model calculates the thermodynamic driving force for a phase.

- **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.



For an example of a driving force model, see example 12 in [Graphical Mode Examples](#).

5.2.5 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 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.

Select the **Matrix phase** and **Precipitate phase** to return the interfacial energy [J/m²].



For an example of an interfacial energy model, see example 11 in [Graphical Mode Examples](#)

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:

$$\text{Eq. 1} \quad \sigma_c = \frac{n_s z_s}{N_A z_l} \Delta E_s$$

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.

Reference

Becker, R., Die Keimbildung bei der Ausscheidung in metallischen Mischkristallen, *Ann. Phys.* 424, 128–140 (1938).

5.2.6 Coarsening Model

The **Coarsening** model calculates the coarsening rate coefficient K (m³/s) of a spherical precipitate phase in a matrix phase.

- **Matrix phase:** Choose the **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.



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 example 11 in [Graphical Mode Examples](#).

Particle Coarsening

In the coarsening regime where the driving force is capillarity, the change of mean particle radius evolves according to the equation:

$$\text{Eq. 2} \quad \bar{r}^3 - \bar{r}_0^3 = Kt$$

Following Morral and Purdy, the rate constant of precipitating β phase in a multicomponent α phase is

$$\text{Eq. 3} \quad K = \frac{8\sigma V_m^\beta}{9} \left[\left[c_i^\beta - c_i^\alpha \right]^T [M]^{-1} \left[c_k^\beta - c_k^\alpha \right] \right]^{-1}$$

The mobility matrix M is not the same as the mobilities that can be obtained directly from DICTRA. The M matrix instead corresponds to the L'' matrix as defined by Andersson and Ågren.

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.

$$\text{Eq. 4} \quad K = \frac{8\sigma V_m^\beta}{9} \left[\left[u_i^\beta - u_i^\alpha \right]^T [L''_{jk}]^{-1} \left[u_k^\beta - u_k^\alpha \right] \right]^{-1}$$

The interfacial energy σ is calculated using the extended Becker's model (that also is available as a separate Property Model Calculator model)

References


- Morral, J. E. & Purdy, G. R. "Particle coarsening in binary and multicomponent alloys," *Scr. Metall. Mater.* 30, 905–908 (1994).
- Andersson, J. & Ågren, J. Models for numerical treatment of multicomponent diffusion in simple phases. *J. Appl. Phys.* 72, 1350–1355 (1992).


5.2.7 Equilibrium Model


The **Equilibrium** model calculates the equilibrium for the given conditions. Optionally define additional **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.


5.3 Equilibrium Calculator


An Equilibrium Calculator allows you to set the conditions for, and perform, a calculation. The Configuration window for an Equilibrium Calculator has these tabs ([Figure 22](#)):

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.  Also see [Setting Equilibrium Calculator Conditions](#), [Setting Conditions for Simplified Mode](#), and [Calculating with a Fixed Phase \(Advanced Mode\)](#).

- **Functions:** Define your own quantities and functions, which you then can calculate and plot.  Also see [Calculating and Plotting Functions](#).
- **Options:** Modify numerical settings that determine how equilibria are calculated, as well as how stepping and mapping calculations are performed.

 Also see [Creating Activities and Successors](#) for a list of possible successors and predecessors for this activity. An Equilibrium Calculator that is the successor of another Equilibrium Calculator inherits all the Configuration window settings of the predecessor.

 For an example of how serially coupled Equilibrium Calculators can be used, see example 6 in [Graphical Mode Examples](#).

 The **Options** tab is where you can locally define specific Equilibrium Calculator settings. These are the same settings described in the [Changing Global Settings](#) section, [Calculation \(Equilibrium Calculator\)](#).

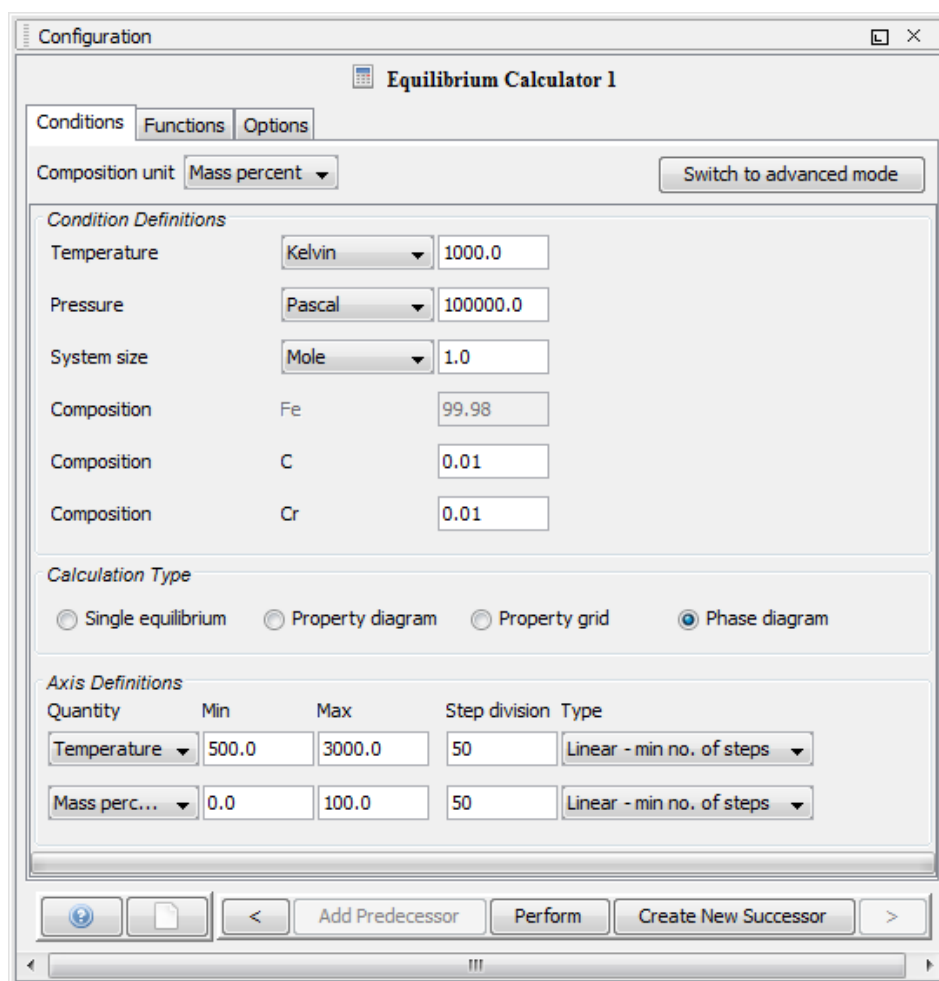



Figure 22: An example of an Equilibrium Calculator Configuration window.

5.3.1 Setting Equilibrium Calculator Conditions

Conditions and axis variables for the Equilibrium Calculator are set in the Conditions tab of the Configuration window ([Figure 22](#)). The tab can be viewed in two modes: simplified (the default) or advanced.

 The conditions to set depend on the type of calculation. For examples of how to set up different calculations, see [Graphical Mode Examples](#):

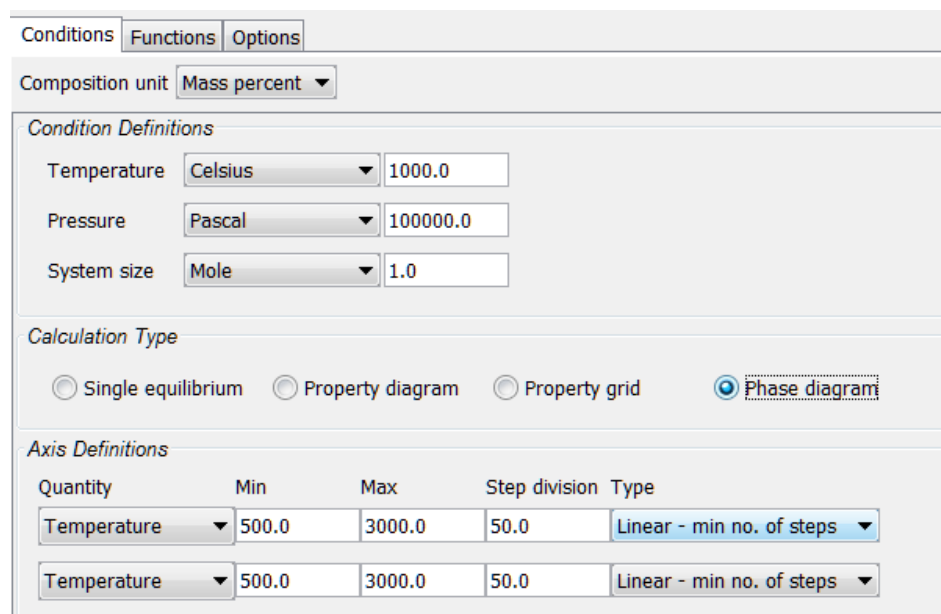
- Example 1 is a single-point equilibrium calculation;
- Example 2 is a stepping calculation;

- Example 5 is a mapping calculation.

In advanced mode, you can 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** 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.


5.3.2 Setting Conditions for Simplified Mode

The following table briefly describes what you can set on the **Conditions** tab in simplified mode. Click **Switch to advanced mode** for more options.



Conditions Tab, Simplified Mode Settings

Setting or condition	Options
Composition unit	Choose from Mass percent , Mole percent , Mass fraction or Mole fraction
<i>Condition Definitions</i>	Specify the values (and units) of the state variables: Temperature , Pressure , and System size .
<i>Calculation Type</i>	Single equilibrium (no axes), Property diagram , Property grid or Phase diagram . For the Single calculation type no further settings are required. The results from this calculation are displayed in the Event Log .
<i>Axis Definitions</i>	Property diagram : Define the axis variable using these fields and menus: Quantity , Min , Max , Step division and Type . Property grid : Define the two axis variables using these fields and menus: Quantity , Min , Max and Number of steps .

Setting or condition	Options
	<p>Phase diagram: Define the two axis variables using these fields and menus: Quantity, Min, Max, Step division and Type.</p> <p> 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.</p>
Number of steps (Property 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 (Property diagram and Phase diagram)	<p>Type options: Linear - min no. of steps, Linear - max step size and Logarithmic - scale factor.</p> <p>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.</p> <p>For Linear - max step size, the Step division sets the maximum size of each step.</p> <p>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.</p>

5.3.3 Calculating with a Fixed Phase (Advanced Mode)

This section 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.

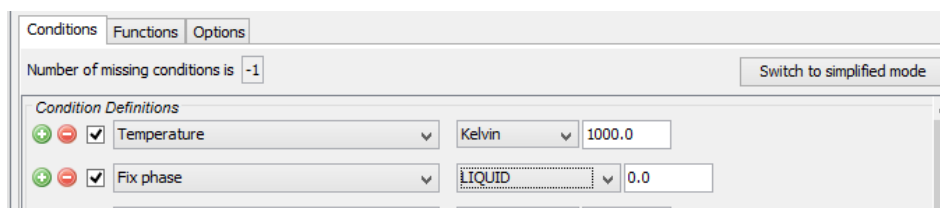
1. Right-click a node that can add an Equilibrium Calculator to your project. See [Creating Activities and Successors](#) for a list.
2. In the **Project** window, click the **Equilibrium Calculator** activity node.
3. In the **Configuration** window, click **Switch to advanced mode** ([Figure 22](#)).




If the **Default calculation mode** is globally set to **Advanced** then by default the Configuration window is already in advanced mode.

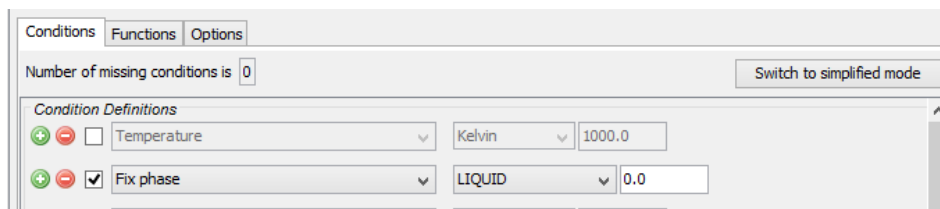
 Also see [Changing Global Settings](#).

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 check-box. 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 **Number of missing conditions is** field displays **0**. When you have set all your conditions, you can perform the Equilibrium Calculator (now or later).

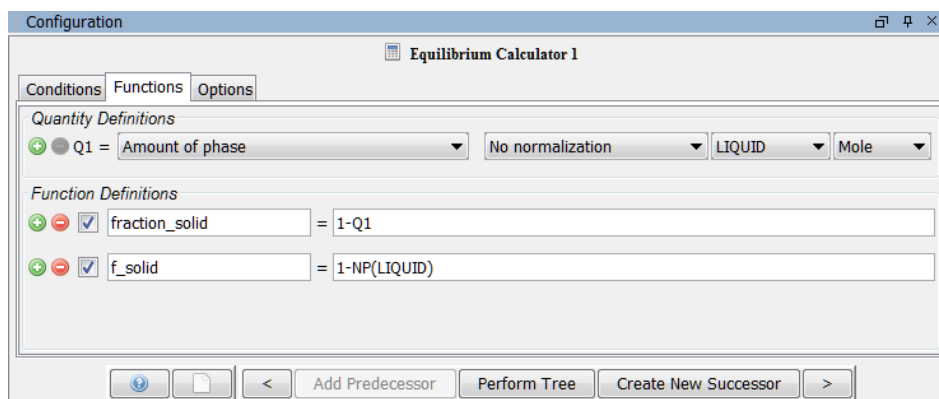
5.3.4 Calculating and Plotting Functions


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 yourself define, see example 7 in [Graphical Mode Examples](#).

1. Create 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.

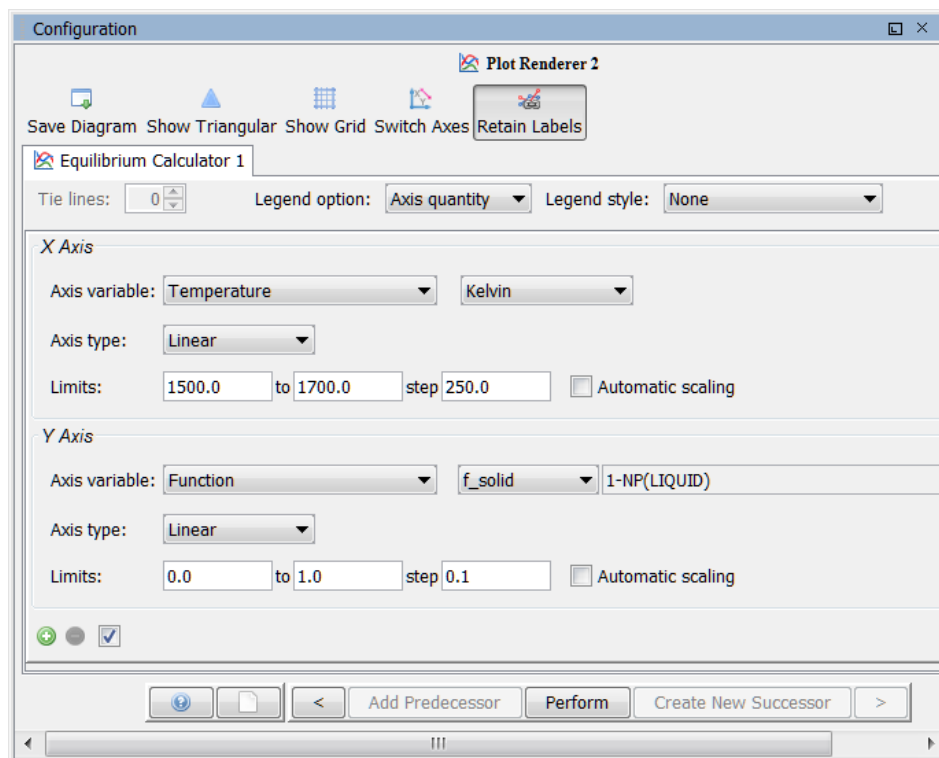


4. Under **Function Definitions**, click the add  button to add a new function. In the left field edit the default name of each function and enter the function itself in the right field after the equal sign. In this example, the quantity defined as Q1 is renamed to **fraction_solid**, which gives as 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)`.

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.




5.4 Plot Renderer

The Plot Renderer displays results from the various calculator activities (Equilibrium Calculator, Property Model Calculator, Binary Calculator, Ternary Calculator, and Scheil Calculator).

The available Plot Renderer functionality varies by calculation type. For example:

- For a Property Grid calculation type or a Plot Renderer Grid calculation type, you choose a **Plot type: Contour** or **Heat map**.
- For a Property Model Calculator Uncertainty calculation type, you choose an **Axis type: Frequency, Histogram** or **Normal probability**. For other calculators (e.g. Equilibrium, Binary, and Scheil) there are different **Axis types** available such as **Linear, Logarithmic, Logarithmic 10** and **Inverse**.

The Plot Renderer is used to set the plotting axis variables for a *property diagram* and *phase diagram*. If you are plotting a *Property grid* (Equilibrium Calculator) or *Grid* (Property Model Calculator) then the X- and Y-axes always represent the quantities that define the stepping 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).

 Also see [Creating Activities and Successors](#) for a list of possible successors and predecessors for this activity. The configurations that can be set in the Configuration window for a Plot Renderer vary depending on the kind of predecessor it is created from.

Plot Several Calculations in One Diagram

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.



For an example of a project in which several calculations are plotted in one diagram, see example 5 in [Graphical Mode Examples](#).

Several Plot Renderer activities (as well as Table Renderer activities) can be shown in the Results window as different tabs as in [Figure 23](#) (from example 4 in [Graphical Mode Examples](#)).

 Also see [Plotting Several Calculations in One Diagram](#).

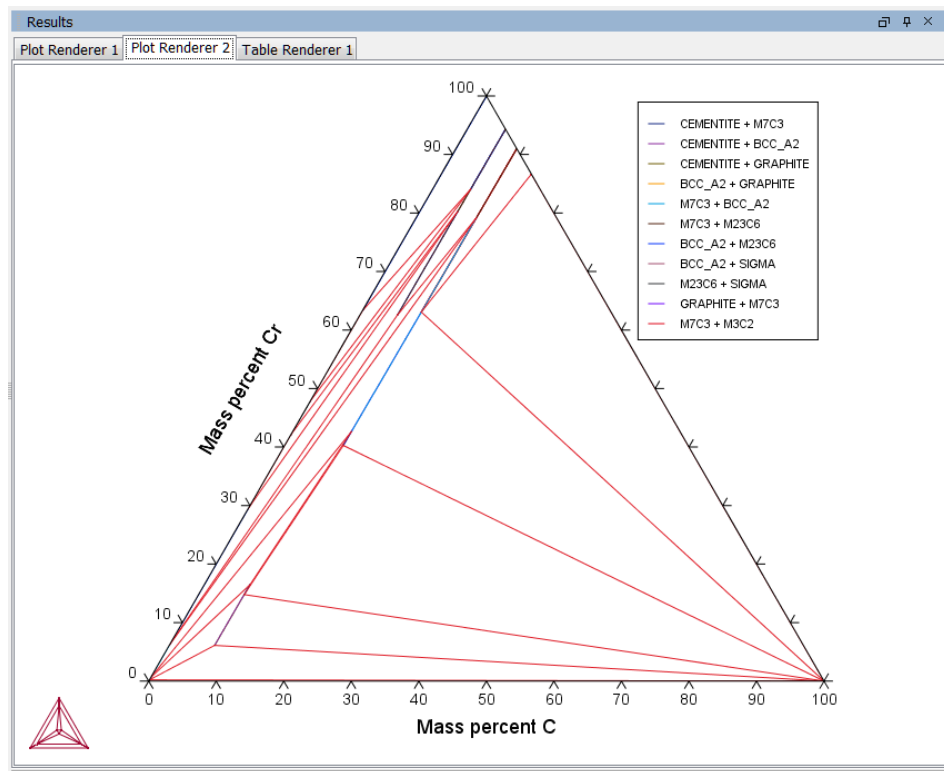


Figure 23: Multiple tabs can be viewed in the Results window.

Add Axes to Diagrams

You can add additional X- and/or Y-axes to a plot to compare two or more variables at the same time as in [Figure 24](#).

👁 Also see [Adding Axes to a Diagram](#).

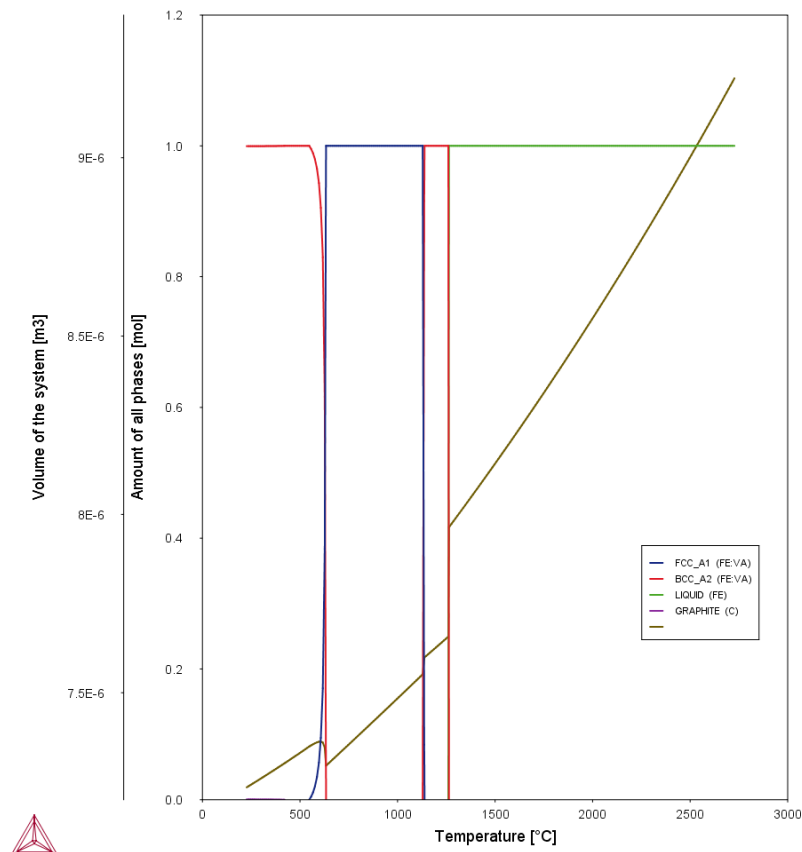


Figure 24: Two variables plotted on the Y-axis.

Merge Results in One Diagram

You can merge (or overlay) calculated results for several variables into one diagram. 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 [Figure 25](#) (from example 12 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).

 Also see [Merging Plots into One Diagram](#) for details of how to combine diagrams.

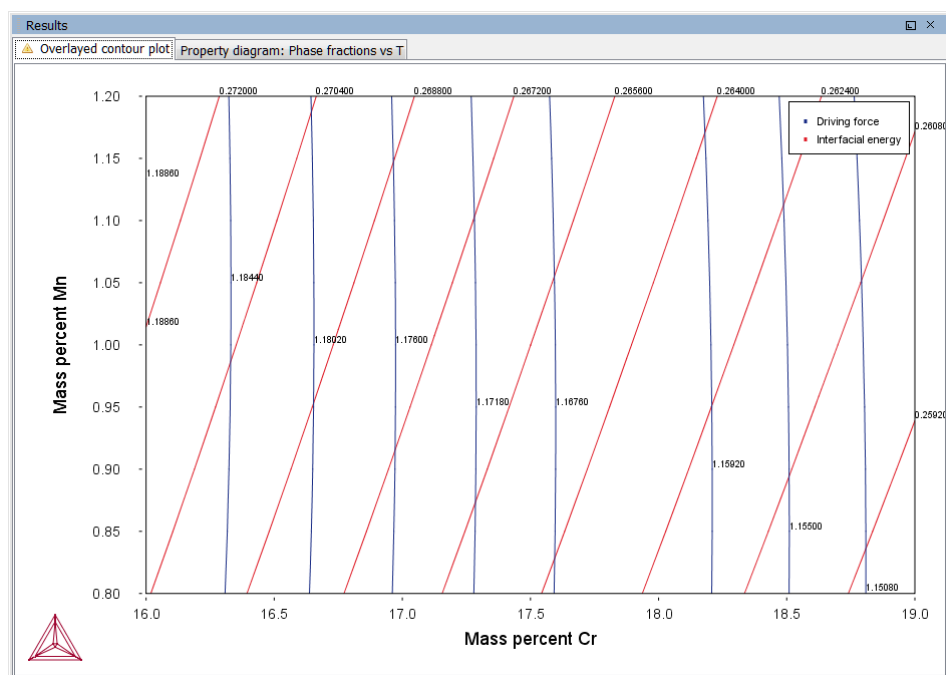
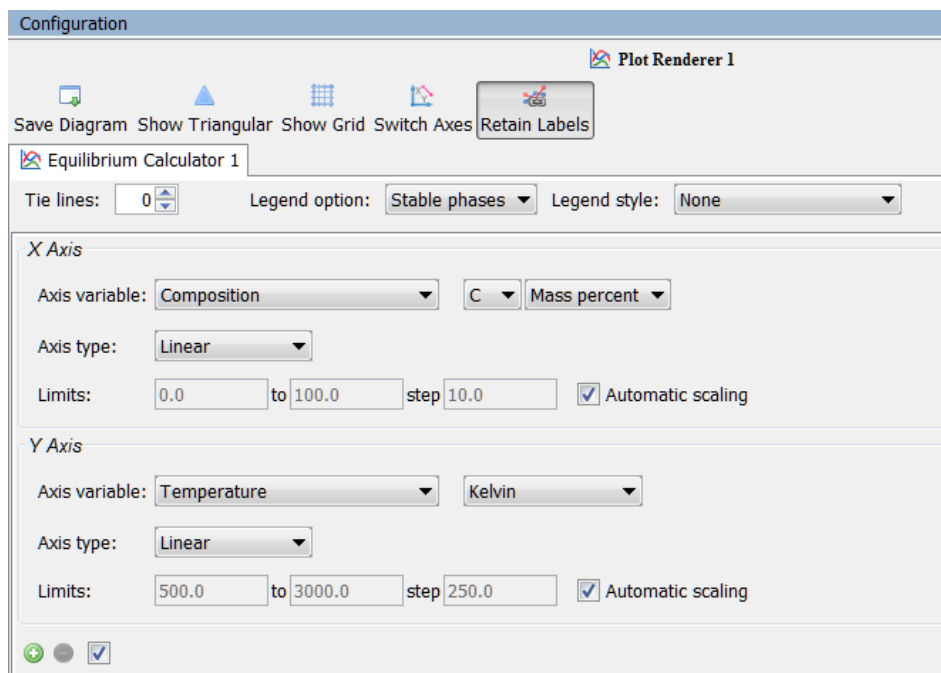









Figure 25: A contour plot showing both the driving force and interfacial energy calculation results comparing Mass percent Cr to Mass percent Mn.





5.4.1 Plot Renderer Configuration Window

The Configuration window has different options available based on its predecessor. The following is an example of the Configuration window for a Plot Renderer that is the successor to an Equilibrium Calculator. The options along the top are available for most of the calculation types (e.g. phase diagrams, property diagrams, min/max, uncertainty and so forth). For an Equilibrium Property Grid calculation type and a Property Model Calculator Grid calculation you can choose a **Plot type**.



Plot Renderer Configuration Settings

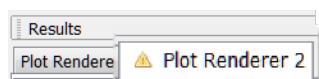
Setting/Button	Description
Save Diagram  Save Diagram	Save the plot diagram.
Show Triangular  Show Triangular	Display the diagram in triangular form, with the X-axis along the base and the Y-axis along the left side. Such a diagram is often useful if you want to plot the fractions of two components in a ternary diagram.
Show Grid  Show Grid	Overlay a grid on the diagram.
Switch Axes  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  Retain Labels	Toggle the default to keep labels displaying on the plot. By default labels are retained.
Tie lines	<p>Select how many tie lines to be plotted in the diagram. Every nth 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.</p> <p> This setting is not available if the Plot Renderer is a successor to a Scheil Calculator or to an Equilibrium Calculator where only one axis is defined and varied (that is, an Equilibrium Calculator that has performed a stepping calculation).</p>
Legend option	Select whether the diagram's legend displays the Stable phases , the Axis quantity , or choose Off for no legend.
Legend style	<p>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.</p> <p> Also see About Legend Styles.</p>
Plot type (property grid or grid calculation types only)	<p>This menu is only available if the Plot Renderer is a successor to either an Equilibrium Calculator that is set up to calculate a <i>property grid</i> or a Property Model Calculator that is calculating a <i>Grid</i>.</p> <p>Choose either Heat map or Contour.</p> <p>On a heat map diagram, each equilibrium calculation in the grid is represented by a colour-coded pixel, where dark red represents the highest Z-axis variable value and dark blue represents the lowest Z-axis variable value.</p> <p>On a contour diagram, Z-axis variable values are traced with curves in different colours (in the same way that height values are traced with curves on a topographical map).</p>

Setting/Button	Description
Axis variable	Set which state variable that 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 what type of scale to use on the axis. Options are based on calculation types. Choose between Linear , Logarithmic , Logarithmic 10 , Inverse , Probability , or Histogram .
Limits	Specify the range along the axis that is shown in the plot by setting the minimum and maximum values of the axis variable. You can also determine the step size between the tick marks along each axis. Alternatively, select Automatic scaling .
Add an axis  and Remove this axis  buttons.	Use these 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.  Also see Adding Axes to a Diagram and Merging Plots into One Diagram for details.

Plot 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 sign—an exclamation mark enclosed in a yellow triangle—is shown in the Plot Renderer's tab.

 Also see [Node Status Markers](#).



5.4.2 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`.

 Also see the *Thermo-Calc Console Mode Command Reference Guide*.

In Graphical Mode the label styles are defined when using the Plot Renderer. 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 Examples

To show the differences between labels, the following uses the same example file that creates Figure 6 in TCNi8 database extended information document (found on the Thermo-Calc website http://www.thermocalc.com/media/23650/tcni8_extended_info_formatted_02.pdf).

[Figure 24](#) is a label that shows **All** available detail as follows:

- 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).

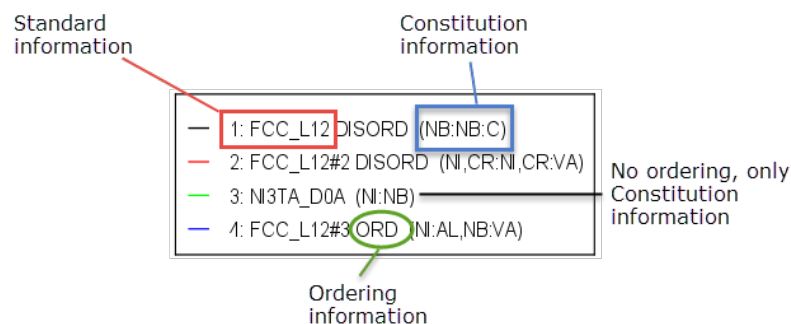


Figure 26: An example of when All is selected to display all information.

The following examples are for each label style choice. 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`.

When **None** is selected the legend includes the standard information about the phases.

—	1: FCC_L12
—	2: FCC_L12#2
—	3: Ni3TA_D0A
—	4: FCC_L12#3

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 (Ni,CR:Ni,CR:VA)
—	3: Ni3TA_D0A (Ni:NB)
—	4: FCC_L12#3 ORD (Ni:AL,NB:VA)

When you select **Constitution description**, this is added to the standard description.

—	1: FCC_L12(NB:NB:C)
—	2: FCC_L12#2(Ni,CR:Ni,CR:VA)
—	3: Ni3TA_D0A(Ni:NB)
—	4: FCC_L12#3(Ni:AL,NB:VA)

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: Ni3TA_D0A
—	4: FCC_L12#3 ORD

5.4.3 Adding and Editing Plot Labels

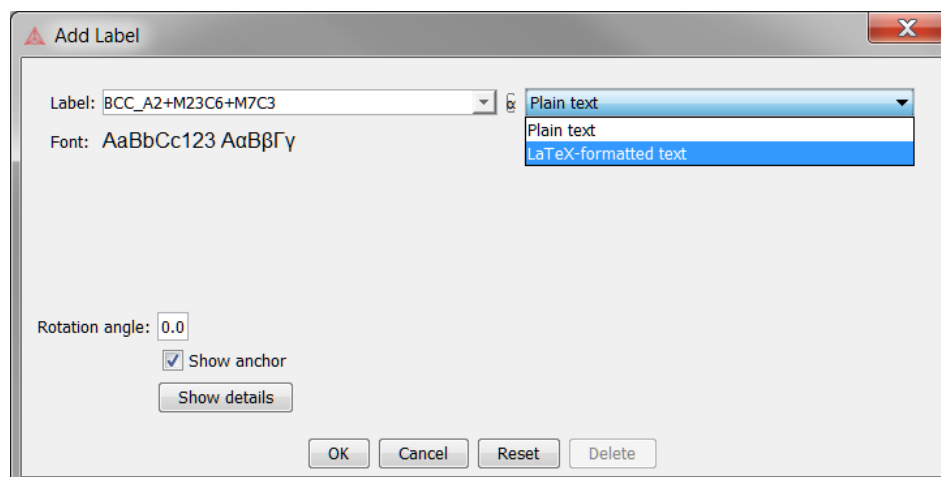
To add a label text at a certain point in a plot, right click the point, and select **Add Label**.

You can enter the label as **Plain text** or in **LaTeX-formatted text**. For **LaTeX-formatted text** the chosen point name is added by default. Use the LaTeX math text to 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>



The suggested label specifies the names of the stable phases at the coordinate where you clicked. 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 the labels by clicking and dragging it. The default anchor arrow is added to indicate the point that belongs to the label.

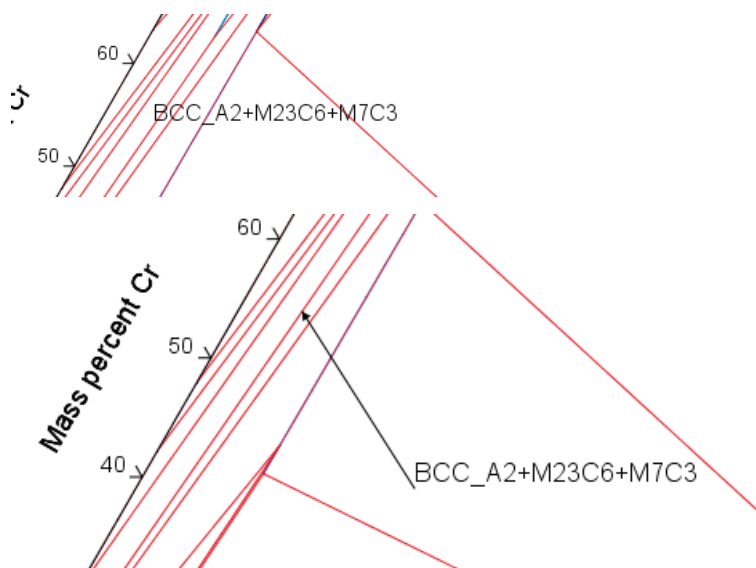



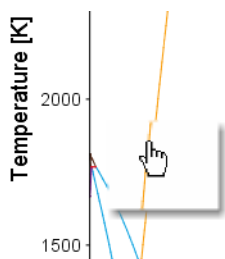
Figure 27: Drag and drop labels anywhere on the plot. The anchor arrow points to the point of origin.


5.4.4 Changing the Plot Properties

 For global changes to the default settings plots see [Graphical and Console Mode-Plotting](#). 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).

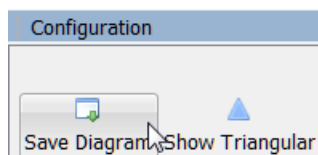
In the **Results** window, hover the mouse over a plot line. When it is over a line that can be clicked the crosshair cursor turns into a pointing finger.



 To prevent unintended edits, hold down <Ctrl> while moving the cursor around the plot to only display it as a crosshair.

5.4.5 Saving Plots

1. To save a diagram, at the top of the **Configuration** window click **Save Diagram**.



Or right-click the diagram in the **Results** window and select **Save As**.

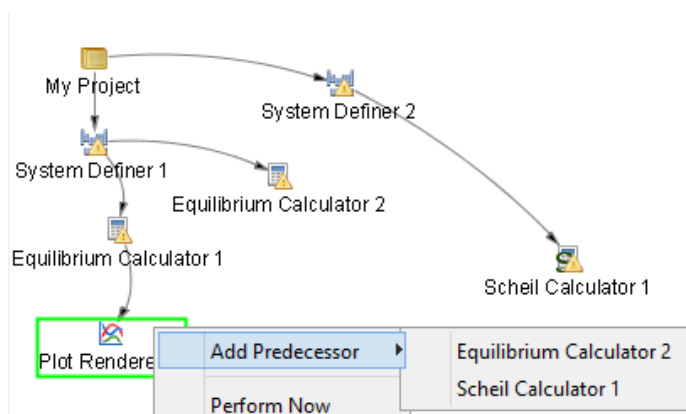
2. In the **Save** window, navigate to where you want to save the plot, enter a **File name**, and choose the **File type** to save it in. Click **Save**.

5.4.6 Plotting Several Calculations in One Diagram

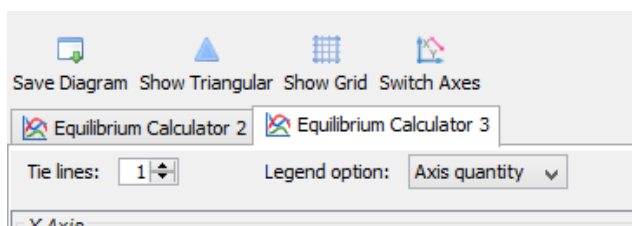
You can plot several calculations in the same diagram by adding extra predecessors to the Plot Renderer activity.

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. The extra predecessor can be any of these: 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**.

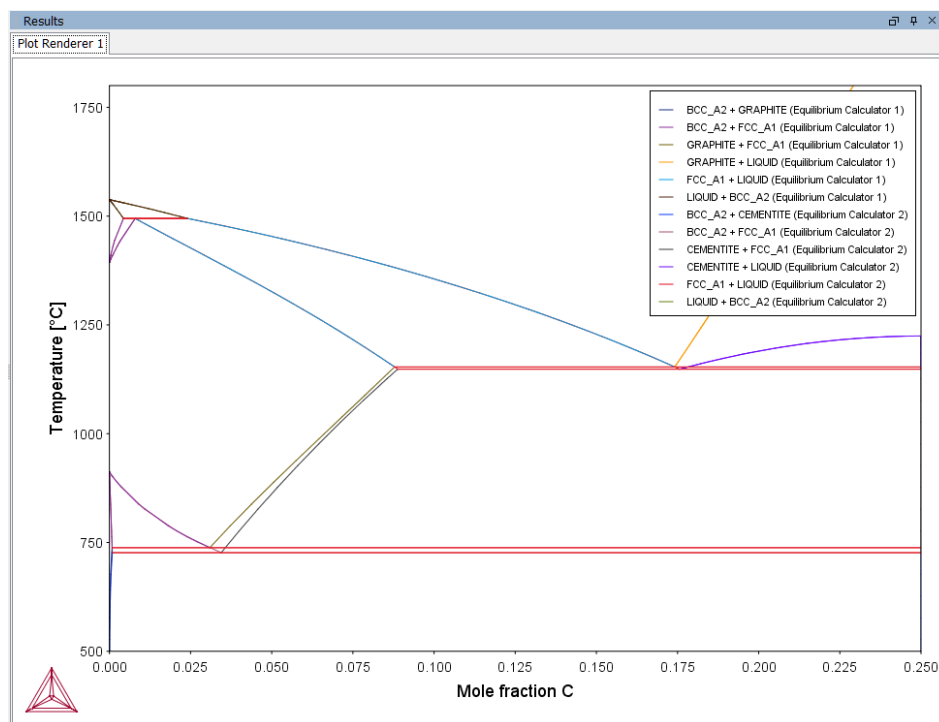


3. Select a predecessor. When added, the extra predecessor is linked to the Plot Renderer. On the Plot Renderer's Configuration window, the predecessors are shown as two tabs:



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.

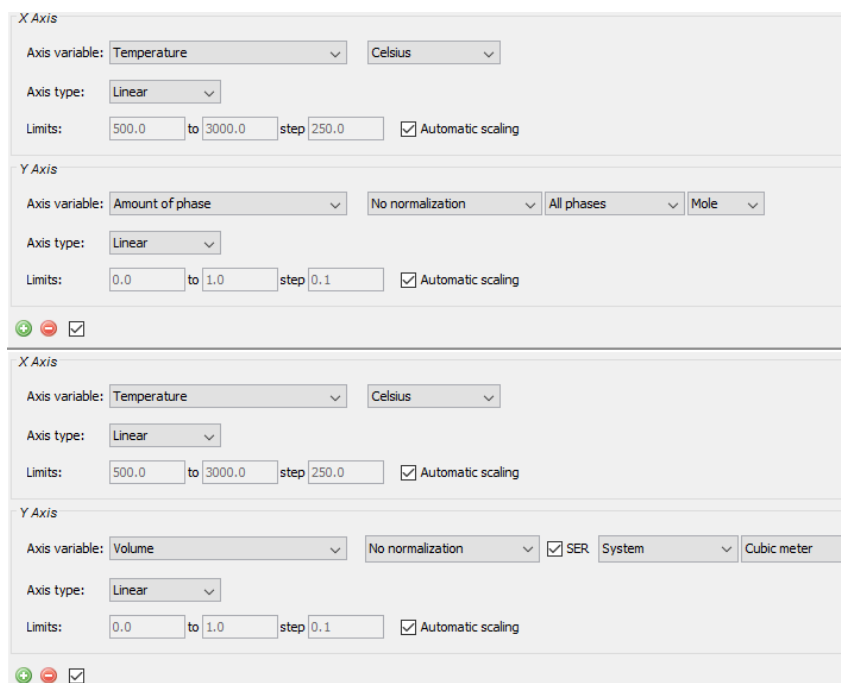


5.4.7 Adding Axes to a Diagram

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 axes settings section is added underneath.
5. From the *X Axis* and/or *Y Axis* sections define another **Axis variable** and choose an **Axis type**. In this example **Amount of phase** and **Volume** are selected as the Y-axis variables and **Temperature** for the X-axis.



The screenshot displays the 'Add an axis' dialog box in Thermo-Calc, showing two separate axis configuration sections. Each section has an 'X Axis' and a 'Y Axis' sub-section.

Top Axis Configuration:

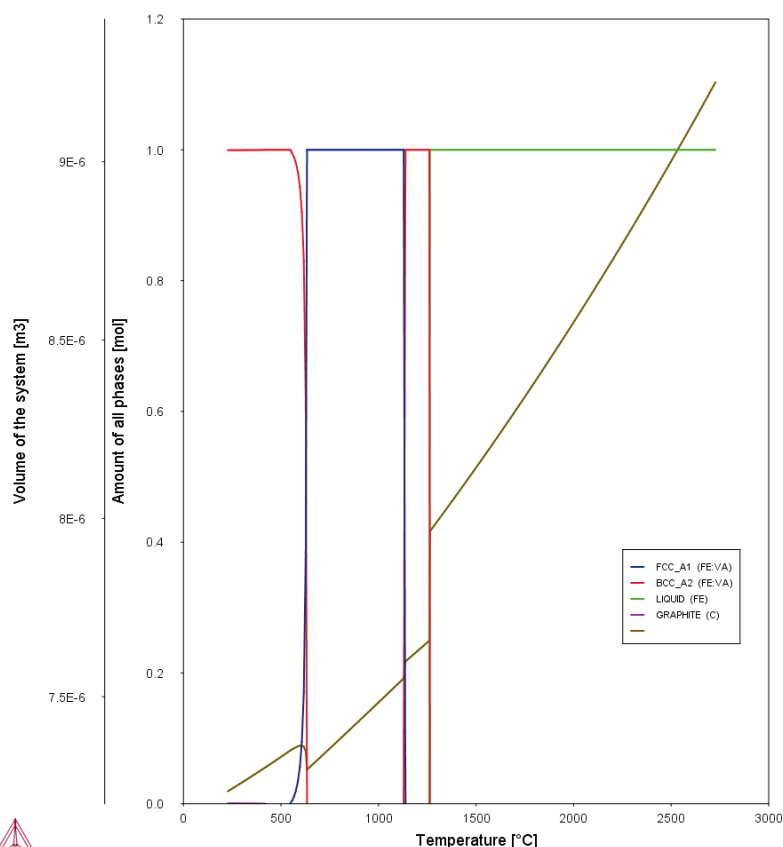
- X Axis:**
 - Axis variable: Temperature
 - Unit: Celsius
 - Axis type: Linear
 - Limits: 500.0 to 3000.0 step 250.0
 - ☒ Automatic scaling
- Y Axis:**
 - Axis variable: Amount of phase
 - Normalization: No normalization
 - Phases: All phases
 - Unit: Mole
 - Axis type: Linear
 - Limits: 0.0 to 1.0 step 0.1
 - ☒ Automatic scaling

Bottom Axis Configuration:

- X Axis:**
 - Axis variable: Temperature
 - Unit: Celsius
 - Axis type: Linear
 - Limits: 500.0 to 3000.0 step 250.0
 - ☒ Automatic scaling
- Y Axis:**
 - Axis variable: Volume
 - Normalization: No normalization
 - ☒ SER
 - System: System
 - Unit: Cubic meter
 - Axis type: Linear
 - Limits: 0.0 to 1.0 step 0.1
 - ☒ Automatic scaling

At the bottom of each configuration section are three buttons: a green plus icon (Add), a red minus icon (Remove), and a checkmark icon (Apply/OK).

6. Click **Perform** to plot both variables on the selected axis.



5.4.8 Merging Plots into One Diagram

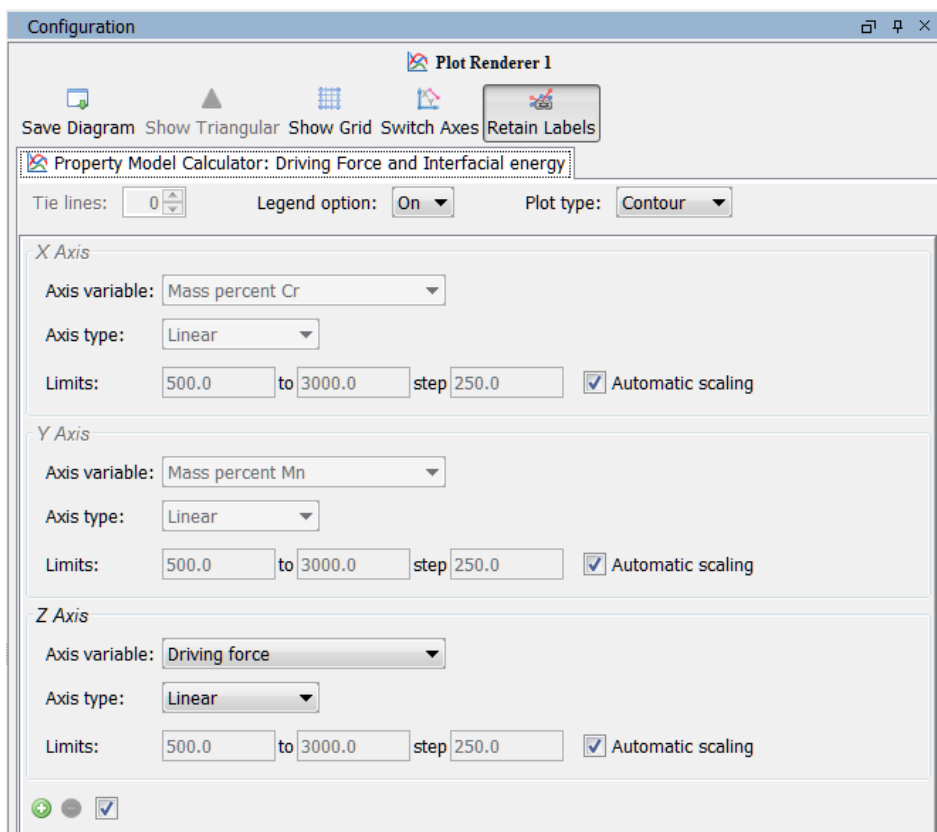
You can merge (or overlay) calculated results for several variables into one diagram. The same X and Y variables are used to compare the third variable (defined in the Plot Renderer as the Z-axis).


 You cannot overlay heat map or frequency plots.

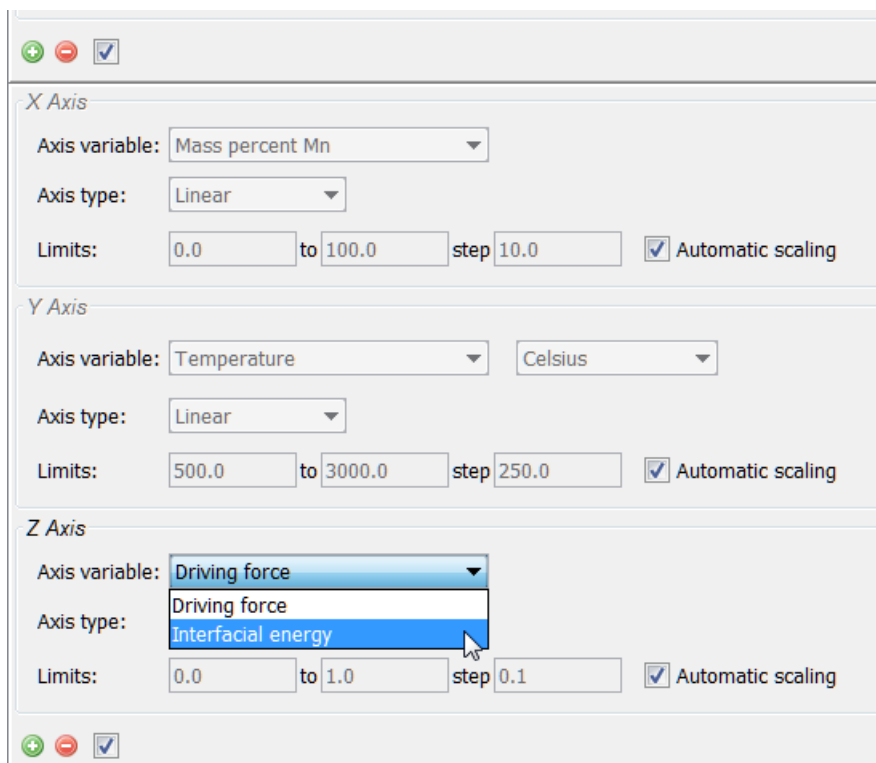
The following uses example 12 in [Graphical Mode Examples](#) to describe the steps to overlay two plots: the driving force and interfacial energy results are combined into one diagram. The X and Y axis is the same for both (Mass percent Cr/Mass percent Mn).

1. In the **Project** window right-click the calculator node (e.g. a 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.

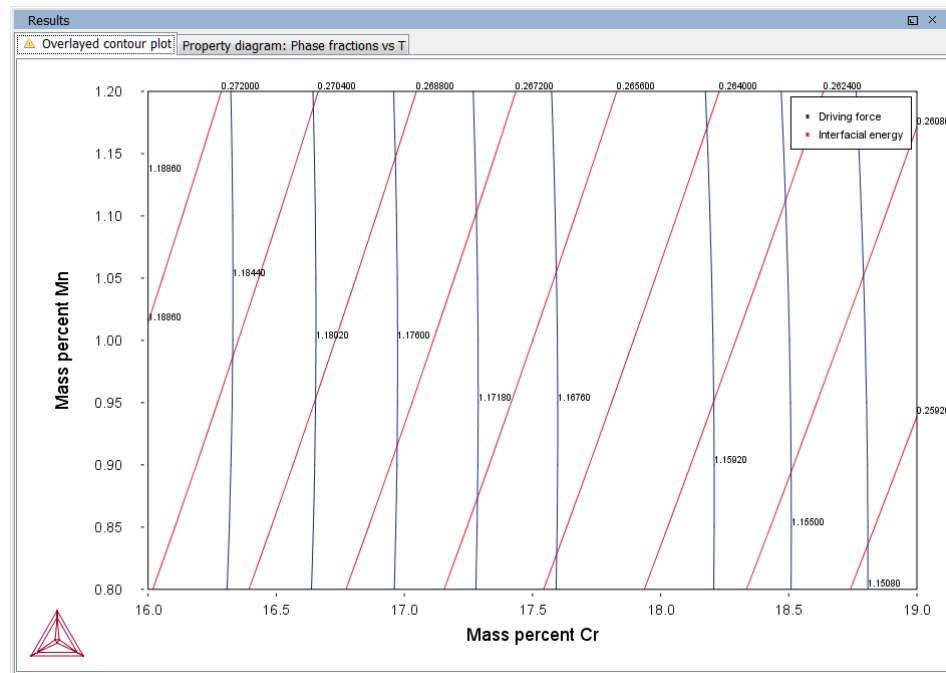
In this example the Property Model Calculator is set to a **Grid** calculation type. Choose **On** for the **Legend option** and **Contour** as the **Plot type**.



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.



5.5 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 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.

 Also see [Creating Activities and Successors](#) for a list of possible successors and predecessors for this activity.

5.5.1 Tabulated Results from an Equilibrium Calculation

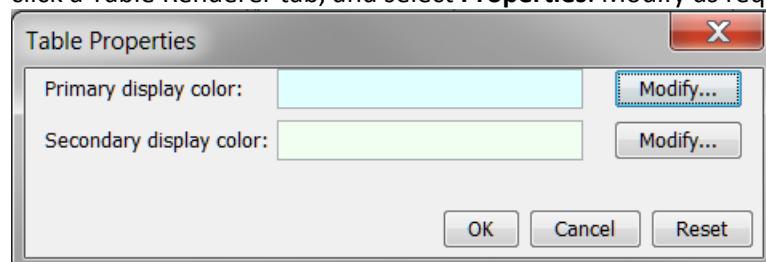
The following tab shows the result of an equilibrium calculation (from example 1 in [Graphical Mode Examples](#)).

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**.

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.




5.5.2 Tabulated Results from a Stepping Operation

The **Table Render 1** tab in the example shows the results of a stepping calculation (from example 2 in [Graphical Mode Examples](#)).

Results				
Plot Renderer 1 Table Renderer 1				
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	

5.5.3 Table Renderer Configuration Window Settings

 Save table

Decimal digits:

Number format:

Columns

☒ Temperature

☒ Amount of phase

Defining the Table Columns

In the **Configuration** window for the Table Renderer 1 node, set the level of detail for the Columns:

Setting Number Format and Number of Decimal Digits

The table results can be presented in ordinary decimal number format or with normalized scientific notation. The **Number format** menu defaults to **Auto** to use the most appropriate format based on the tabulated data. Or choose **Scientific** or **Decimal** to increase or decrease the number of **Decimal digits** used in the table.

Saving Tabulated Data

To save all the data in a table as a plain text file, 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. If data is calculated but not displayed it is not saved.

5.6 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. For more information about DATAPLOT search the online help or refer to the *DATAPLOT User Guide*.



Also see [Creating Activities and Successors](#) for a list of possible successors and predecessors for this activity.

5.6.1 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.
3. Click **Create New Successor** and select **Plot Renderer**. Or right-click the **Experimental File Reader** node and from the **Create New Successor** submenu choose **Plot Renderer**.
4. In the **Configuration** window click **Perform** or right-click the **Plot Renderer** node and select **Perform**.

5.7 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.

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 example 3 in [Graphical Mode Examples](#).



Also see [Creating Activities and Successors](#) for a list of possible successors and predecessors for this activity.

5.7.1 Binary Calculator Configuration Window

The following shows the **Configuration** window of a **Binary Calculator** activity:

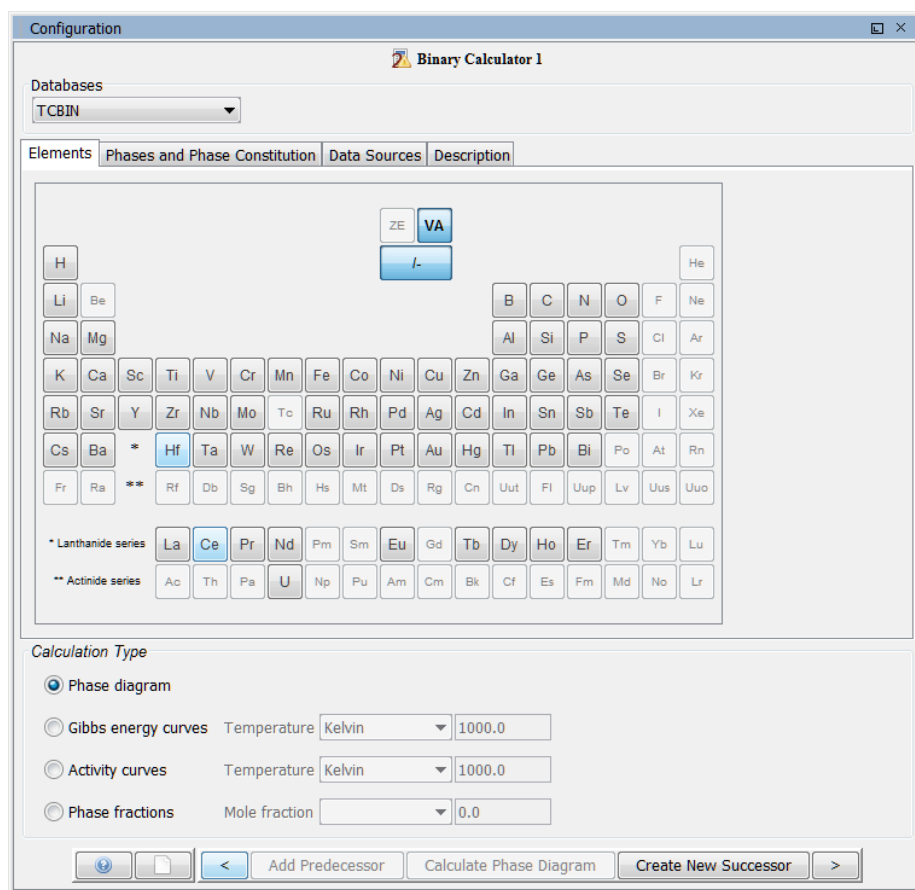


Figure 28: An example of a Binary Calculator Configuration window.

The table lists the available settings to configure before performing the calculation.

Binary Calculator Configuration Settings

Setting	Description
Select database	Select a database that contains specifications dedicated to the Binary Calculator.
Elements (periodic table)	In the periodic table, select the two elements that make up the components of the system.
Phases and Phase Constitution	This tab is the same as for a System Definer . 👁 Also see Phases and Phase Constitution for an example.
Data Sources	This tab is the same as for a System Definer . 👁 Also see Data Sources for an example.
Description	This tab is the same as for a System Definer . 👁 Also see Description for an example.
Calculation Type	
Phase diagram	Select to perform a mapping calculation. Click Calculate Phase Diagram to plot the results.

Setting	Description
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.

5.8 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.



For an example of how a Ternary Calculator is used in a project, see example 4 in [Graphical Mode Examples](#).



Also see [Creating Activities and Successors](#) for a list of possible successors and predecessors for this activity.

5.8.1 Ternary Calculator Configuration Window

The following shows the Configuration window of a Ternary Calculator activity:

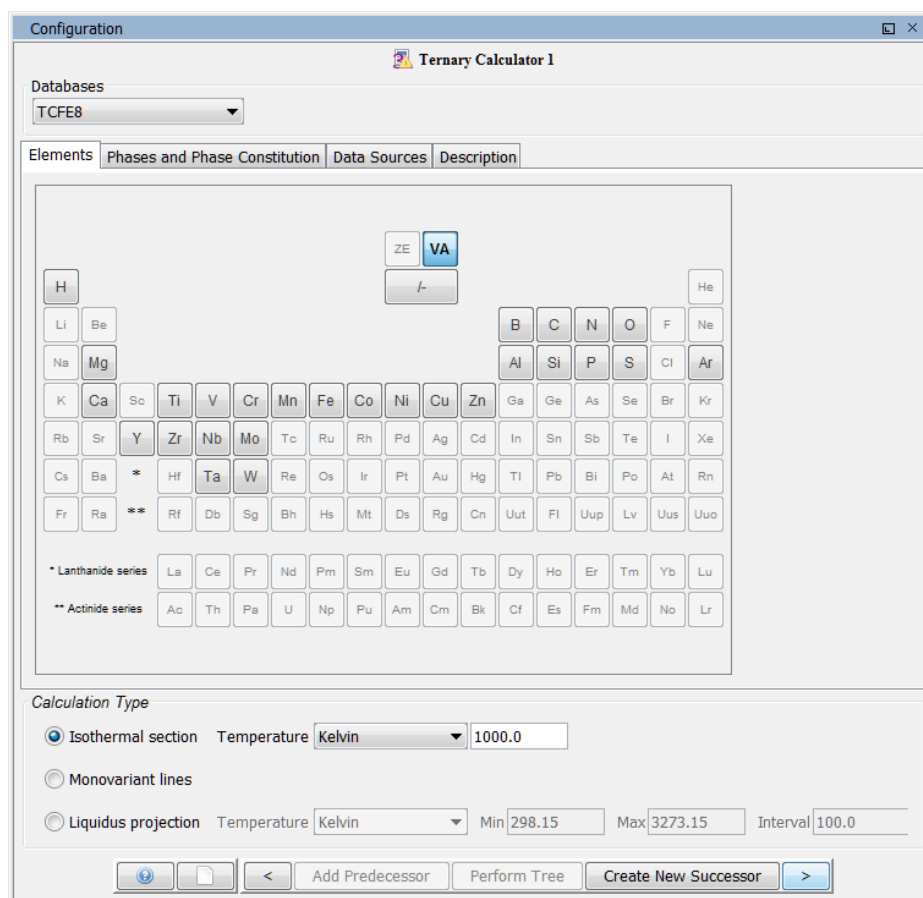


Figure 29: An example of a Ternary Calculator Configuration window.

The table lists the available settings that must be configured before performing the calculation.

Ternary Calculator Configuration Settings

Setting	Description
Select database	Select a database that contains specifications dedicated to the Ternary Calculator.
Elements (periodic table)	In the periodic table, select the three elements that make up the components of the system.
Phases and Phase Constitution	This tab is the same as for a System Definer . 👁 Also see Phases and Phase Constitution for an example.
Data Sources	This tab is the same as for a System Definer . 👁 Also see Data Sources for an example.
Description	This tab is the same as for a System Definer . 👁 Also see Description for an example.
Calculation Types	
Isothermal section	Select the Temperature at which the ternary system is calculated for the whole composition range.

Setting	Description
Monovariant lines	The variation of the liquid compositions with temperature is calculated.
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.

5.9 Scheil Calculator

The Scheil Calculator activity is used to perform simulations of *Scheil (Scheil-Gulliver) solidification processes*. By default, a Scheil calculation results in an estimation of the solidification range of an alloy. The calculation is based on the assumption that the liquid phase is homogeneous at all times and that the diffusivity is zero in the solid. However, it is possible to disregard the latter assumption for selected components.



See example 8 in [Graphical Mode Examples](#).



Also see [Creating Activities and Successors](#) for a list of possible successors and predecessors for this activity.

By default, a Plot Renderer successor 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.



Also see [Scheil Simulations](#) in the Console Mode section.

5.9.1 Scheil Calculator Configuration Window

The main **Configuration** window of a **Scheil Calculator** activity is shown below and listed in the table. These settings must be configured before performing the calculation.

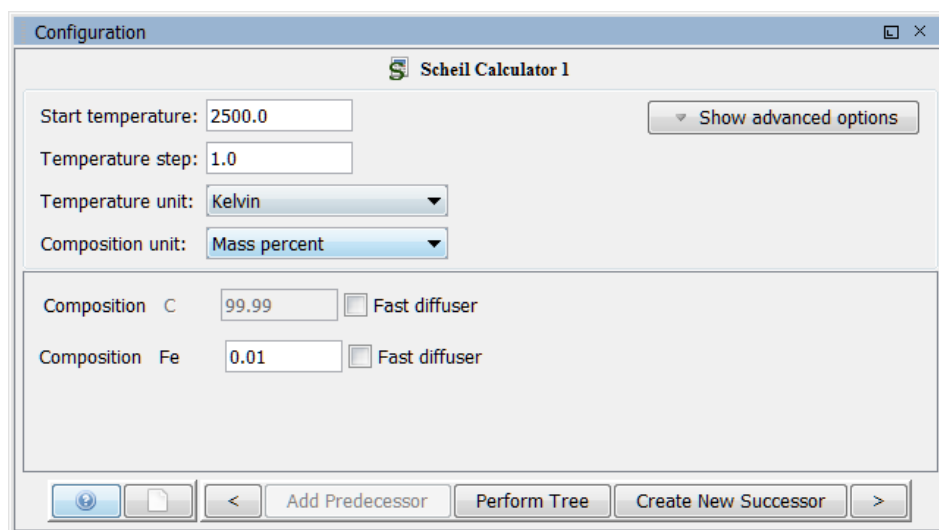


Figure 30: An example of a Scheil Calculator Configuration window.

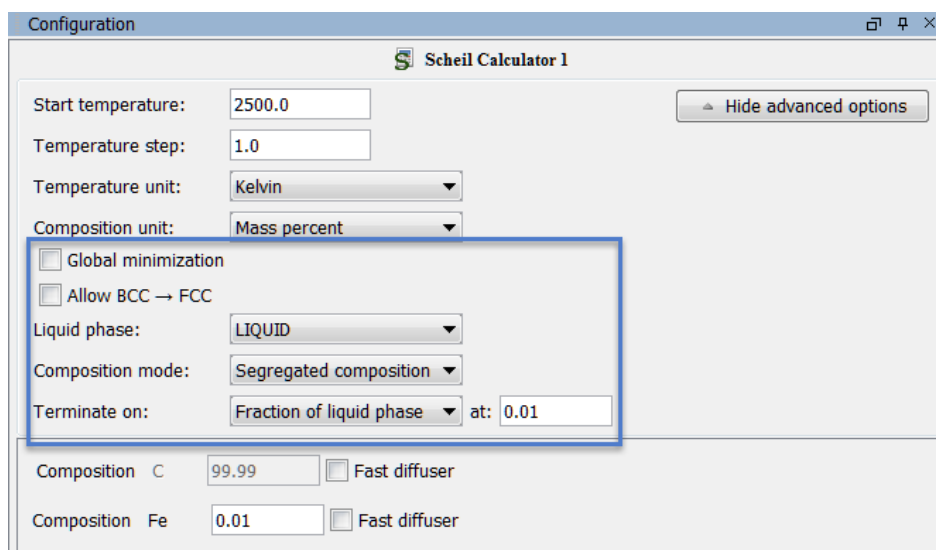
Scheil Calculator Configuration Settings

Setting	Description
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.
Composition	This is based on what is entered in the System Definer .
Fast diffuser	Click to select the Fast diffuser check box to allow redistribution of this component in both the solid and liquid parts of the alloy.

Scheil Calculator Advanced Options

Additional advanced settings are available as shown below and in the table:

Click **Show advanced options** to open this configuration window:



Scheil Calculator Advanced Settings

Setting	Description
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.
Allow BCC → FCC	By default the Allow BCC→ FCC check box is not selected. Select the check box to allow transformations in the solidified part of the alloy caused by each of the components specified to be a <i>fast diffuser</i> . It is recommended that you only select this for steels.

Setting	Description
Liquid phase	The default in the list is the Liquid phase already defined in the database.
Composition mode	<p>Use this setting to choose the composition type (the mode) to store for post processing. This must be chosen before performing a simulation.</p> <p>The results of a Scheil Calculator activity are stored in the same workspace as the standard POLY-3 calculations. There are two composition types, <i>segregated</i> or <i>average</i>, that can be stored in this workspace. By default, it is stored in the workspace as a Segregated composition. Choose instead to save it as an Average composition so you can maintain the mass balance and evaluate several other quantities during a simulation.</p>
Terminate on	Enter a value to terminate the calculation on the Fraction of liquid phase or at a specific Temperature .

6. The Console Mode Interface

The following is an introduction to the Console Mode's user interface and the command line prompt.

 Also see [The Graphical Mode Interface](#).

- [The Console Mode Layout](#)
- [Console Window](#)
- [Console Mode Results Window](#)
- [Event Log Window](#)
- [Console Mode Workflow](#)
- [Performing Calculations in Console Mode](#)
- [Using the Command Line Prompt](#)
- [Moving Between Modules and Submodules](#)
- [Entering Command Names or Abbreviations](#)
- [Specifying Parameters](#)
- [Wild Card Characters](#)
- [Controlling Console Output](#)
- [Command History](#)
- [Log, Macro and Workspace Files](#)
- [Log Files](#)
- [Macro Files](#)
- [Workspace Files](#)
- [Main Menu Commands](#)
- [Defining a System in Console Mode](#)

6.1 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.

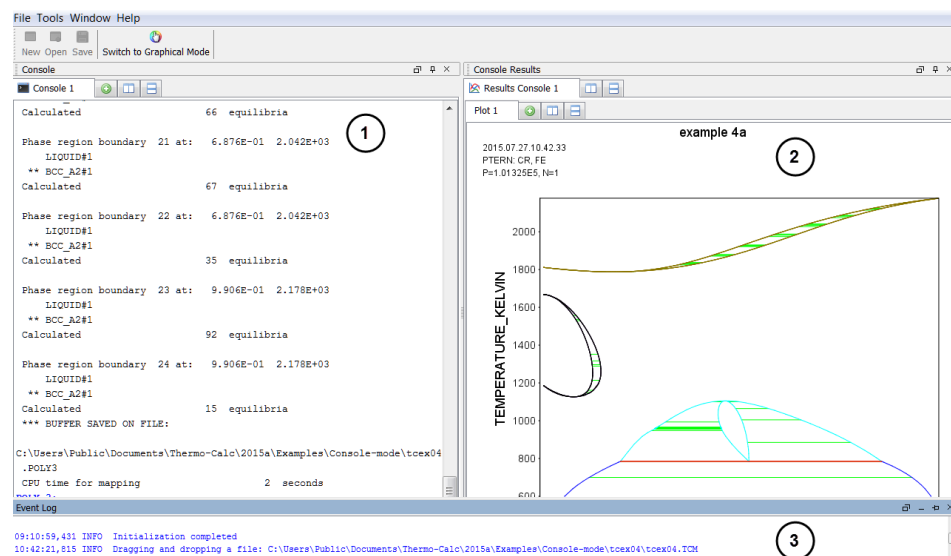
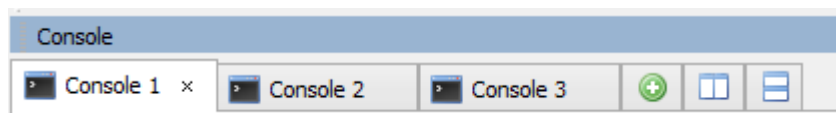





Figure 31: The Console Mode user interface with windows and tabs.

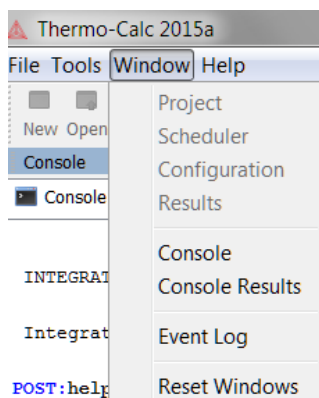
The currently selected window is called the *active* window. This has a darker title bar than the other windows. The windows shown in [Figure 29](#) are:

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.

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 a specific window from the **Window** main menu, or select **Reset Windows** to return to the default window layout.

6.2 Console Window

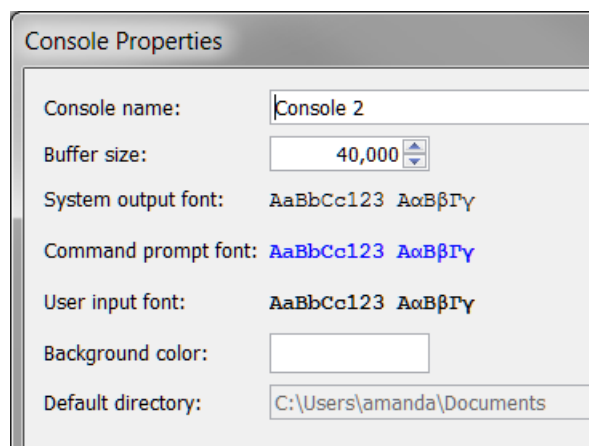
By default the Console window is on the left-hand side of the console. This is where you enter commands. The window can have several Console tabs.

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 colours for an individual Console tab by right-clicking its header and selecting **Properties**.

 Also see [Console Mode-Default Appearance](#).



6.3 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>.

6.4 Event Log Window

By default the Event Log 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.

6.5 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. See [Typical POLY Module Workflow](#). (It is possible to define a system directly in POLY using DEFINE_MATERIAL and DEFINE_DIAGRAM).
- 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.

6.5.1 Typical POLY Module Workflow

[Figure 30](#) represent the typical workflow when you perform calculations in the POLY module. The solid arrows represent your typical movements between the modules. The dashed arrows represent the movement of data within Thermo-Calc.

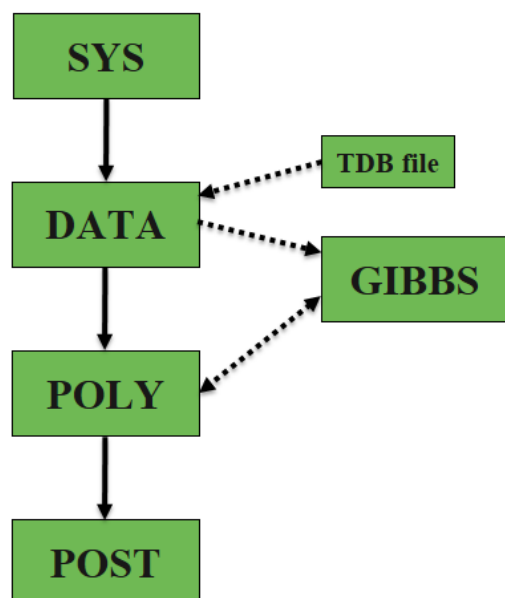


Figure 32: An example of a typical POLY module workflow.

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.

6.6 Performing Calculations in Console Mode

Later in this guide are descriptions of the common calculations performed in Thermo-Calc. Calculations can be performed either in the POLY module, or using some of the response-driven modules designed to perform specific types of calculations.

The [Equilibrium Calculations](#), section describes generally how to calculate and plot [Property Diagrams](#) and [Phase Diagrams](#). To calculate and plot a property diagram or a phase diagram, you must first calculate an equilibrium.

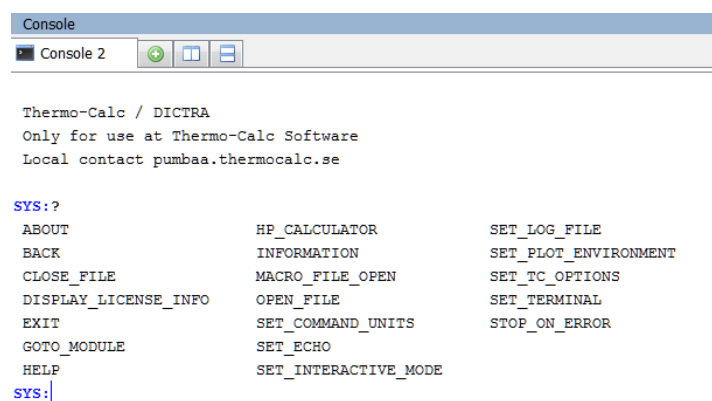
Additional sections discuss [Scheil Simulations](#), [T0 Temperature Simulations](#), [Paraequilibrium](#), [Potential Diagrams](#), and [Aqueous Solutions](#).

 Also search the online help or see [Tabulation of Chemical Substances](#), [Phases or Reactions](#) and the [Thermo-Calc Console Mode Command Reference](#) (the *POLY Commands* section).

6.7 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>`, as in [Figure 31](#).



```

Console
Console 2

Thermo-Calc / DICTRA
Only for use at Thermo-Calc Software
Local contact pumbaa.thermocalc.se

SYS: ?
ABOUT                HP_CALCULATOR        SET_LOG_FILE
BACK                  INFORMATION           SET_PLOT_ENVIRONMENT
CLOSE_FILE            MACRO_FILE_OPEN       SET_TC_OPTIONS
DISPLAY_LICENSE_INFO  OPEN_FILE             SET_TERMINAL
EXIT                  SET_COMMAND_UNITS     STOP_ON_ERROR
GOTO_MODULE           SET_ECHO
HELP                  SET_INTERACTIVE_MODE
SYS:|
  
```

Figure 33: A list of the available SYS module commands.

 Also see:

- [Moving Between Modules and Submodules](#)
- [Entering Command Names or Abbreviations](#)
- [Specifying Parameters](#)

- [Default Parameters Values](#)
- [Wild Card Characters](#)
- [Controlling Console Output](#)
- [Command History](#)

6.8 Moving Between Modules and Submodules

To go to a specific module, you typically use GOTO_MODULE followed by the name of the module. For example, to go to the DATA module, type
GOTO_MODULE 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 if you have DICTRA, from that module.
- To go to the ED-EXP 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 DICTRA license key.

6.9 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 of Command Names and Abbreviations

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-S S-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-S S-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-L S-OU

6.10 Specifying Parameters

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 type `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.

6.10.1 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
```

6.11 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 of Wild Card Characters in Console Mode

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.

Command	Action
SHOW_VALUE W(\$,*)	Lists mass fractions of all components in all stable phases.
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.

6.12 Controlling Console Output

In response to a command Thermo-Calc may display a lot of text in the Console window.

 Also see [Increasing the Buffer Size](#).

- To pause the text on printing press <Ctrl+S>.
- To resume the printing on screen, press <Ctrl+Q>.
- When Thermo-Calc is performing a 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+C>.

6.13 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.

6.14 Log, Macro and Workspace Files

In Console Mode, Thermo-Calc uses different kinds of files, including:

- [Log Files](#) (*.LOG)
- [Macro Files](#) (*.TCM or *.LOG)
- POLY [Workspace Files](#) (*.POLY3),
- Experimental data files (*.EXP) (see the [Data Optimisation User Guide](#) on the website for information).

- The GIBBS module uses a workspace file (*.GES5)
- The PARROT module uses files with the suffixes *.PAR and *.POP.

6.15 Log Files


Log files 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.

 For details about the SET_LOG_FILE and SET_ECHO commands see the [Thermo-Calc Console Mode Command Reference](#) on the website.

6.16 Macro Files

Macro files 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.

 For details about the MACRO_FILE_OPEN command see the [Thermo-Calc Console Mode Command Reference](#) on the website.

 Also see Example 12 in [Console Mode Examples](#).

Action	Command	Description and Comments
To load a macro file	In the SYS module, MACRO_FILE_OPEN 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	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.

Action	Command	Description and Comments
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.

6.16.1 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.


6.16.2 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 POST or the SET_INTERACTIVE command (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).

6.17 Workspace Files


You can save all the data in your current workspace by first using SAVE_WORKSPACES. This command is available in the POLY, GIBBS and PARROT modules. 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 GIBBS. 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.

 For more details about the SAVE_WORKSPACES and READ_WORKSPACES commands search the online help or see the [Thermo-Calc Console Mode Command Reference](#) on the website.

6.18 Main Menu Commands

The **File** menu and toolbar are reserved for Graphical Mode. In Console Mode you use commands to access these menu options. The **Tools**, **Window** and **Help** menus are described in the [Main Menu and Toolbar](#) section. If there is an equivalent command, it is listed in the table below.

 Also search the online help or see the [Thermo-Calc Console Mode Command Reference](#) on the website.

Console Mode Main Menu Commands


Option	Command
Open files	In Thermo-Calc, drag and drop the file into the Console window.

Option	Command
	In the SYS module: MACRO_FILE_OPEN In the SYS module: OPEN_FILE
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 (GIBBS module)
Exit	In any module: EXIT
Close	In the SYS module: CLOSE_FILE
Display license info	In the SYS module: DISPLAY_LICENSE_INFO

6.19 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 DEFINE_MATERIAL and DEFINE_DIAGRAM

 Search the online help or see the [Thermo-Calc Console Mode Command Reference](#) on the website for information about the commands used in this section. See *DATABASE_RETRIEVAL Commands*.

6.19.1 How to Define a System in Console Mode

1. Go to the DATA module. At the SYS prompt, type GOTO_MODULE 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_TCFE8, then the current database is TCFE8.

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 ELEMENTS.) For example, if you want to have Fe and C in your system, type:

```
DEFINE_ELEMENTS Fe C
```

4. Use REJECT 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 PHASES. To list the phases that can form in the

defined system, use LIST_SYSTEM 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 the preceding 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.

7. Equilibrium Calculations

- [About Equilibrium Calculations](#)
- [Calculating an Equilibrium](#)
- [Calculating an Equilibrium with a Fixed Phase](#)
- [Calculating an Equilibrium with Suspended or Dormant Phases](#)

7.1 About Equilibrium Calculations

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 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.

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 ($X(\text{LIQ}, S) - X(\text{PYRR}, S) = 0$).

The number of state variables that needs 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)

The following table lists some of the available state variables you can use to set conditions:

Examples of State Variables for Setting Conditions

State variable	SET_CONDITION parameter
temperature in the system (in K)	T
pressure in the system (in Pascal)	P
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>)

State variable	SET_CONDITION parameter
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>)

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.

Here is an example of the kind of information about the equilibrium normally shown:

```
POLY_3:1-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VMCS/:
  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
```

7.2 Calculating an Equilibrium

This section 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.

1. Define your system (see [Defining a System in Console Mode](#)).
2. Go to the POLY module. At the SYS prompt, type GOTO_MODULE 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.

7.3 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 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 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 Example 7 in [Console Mode Examples](#).

7.4 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 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 Example 10 in [Console Mode Examples](#).

8. Property Diagrams

- [About Property Diagrams](#)
- [Calculating and Plotting a Property Diagram](#)
- [Calculating a Property Diagram One Phase at a Time](#)
- [Calculating Several Properties in the Same Diagram](#)

8.1 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 Example 8 in [Console Mode Examples](#).

8.2 Calculating and Plotting a Property Diagram

This section 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.


1. Calculate an initial equilibrium in the POLY module (see [Equilibrium Calculations](#)).
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 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. By default, the X-axis represents the stepping axis variable and Y-axis represents the sum of the mole fractions of all phases (NP(*)).

8.3 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 ONE_PHASE_AT_TIME to perform the stepping operation.

8.4 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!

9. Phase Diagrams

- [About Phase Diagrams](#)
- [Calculating and Plotting a Phase Diagram](#)
- [Calculating a Quasi-Binary Phase Diagram](#)
- [Calculating a Quasi-Ternary Phase Diagram](#)

9.1 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 describes how to calculate the types of phase diagrams in the POLY 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.




For an example of the calculation and plotting of a phase diagram, see Example 4 in [Console Mode Examples](#).

9.2 Calculating and Plotting a Phase Diagram

This section describes how to calculate a phase diagram in the POLY module.

1. Calculate an initial equilibrium in the POLY module (see [Equilibrium Calculations](#)).
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.

- 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
```

- 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.

- 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
```

- To plot the diagram, use POST to open the POST module and then use PLOT. By default, the X-axis represents mapping axis variable 1 and the Y-axis represents mapping axis variable 2.

9.3 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.

Use `CHANGE_STATUS` to set the component that has a fixed activity or chemical potential. For example, suppose you want to compute a phase diagram for a Ca-Fe-O system in which the liquid oxide (`FE-LIQ`) is in equilibrium with liquid Fe. You then enter:

```
CHANGE-STATUS FE-LIQ=FIX 0
```



For an example of a calculation of a quasi-binary phase diagram, see Example 17 in [Console Mode Examples](#).

9.4 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
```


10. Scheil Simulations

- [About Scheil Simulations](#)
- [Simulating a Scheil-Solidification](#)
- [Plotting Additional Scheil Simulation Diagrams](#)

10.1 About Scheil Simulations

Thermo-Calc is primarily a program for performing equilibrium calculations, but some non-equilibrium transformations or partial-equilibrium transformations can be simulated. One example of such a transformation is a Scheil-Gulliver solidification. In a Scheil-Gulliver solidification, the diffusion in the solid phases is assumed to be so slow that it can be ignored, while the diffusion in the liquid phase is assumed to be very fast. With this approximation, the conditions at the liquid/solid interface can be described as a local equilibrium.

By making a stepping operation on the temperature variable (or enthalpy or amount liquid phase) with small decrementing steps, the new composition of the liquid can be determined. After each step, the amount of formed solid phase is removed and the overall composition is reset to the new liquid composition. In effect, the whole system is described as a non-equilibrium state regarding various parts of solidified phases at various solidification stages.


You can simulate Scheil-Gulliver solidification processes with the SCHEIL module. When you enter the module, you are prompted to answer a series of questions about which database to use, what the major element is and in which amount. 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. Do this by starting a new simulation, by opening an old file with the results of a previous simulation that you can plot differently. 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.


It is possible to use the SCHEIL module to run a modified Scheil-Gulliver simulation that also take back-diffusion of some fast-diffusing interstitial elements such as C or N into account, as well as BCC to FCC phase transformation phenomena.



Also see the *Thermo-Calc Command Reference* and [Console Mode Examples](#) for more information about how to use the SCHEIL module:

- See Examples 15 and 30 to simulate non-equilibrium transformations without considering fast-diffusion elements.
- See Example 48 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).

 If you also have a license for DICTRA, you can import a previously calculated Scheil segregation profile into the software using the command `INPUT_SCHEIL_PROFILE`.

 Search the online help or see the *DICTRA Command Reference*.

10.2 Simulating a Scheil-Solidification

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).

1. Use `GOTO_MODULE SCHEIL` to enter the SCHEIL module.
2. Type `START-WIZARD`.
3. Specify which `Database` to use.
4. Specify the `Major element or alloy` in your system.
For example, for a steel/Fe-alloy, enter `Fe`, for an Al-based alloy, enter `Al`, and for a Ni-based super alloy, enter `Ni`.
5. 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.
6. Specify the name of the `1st alloying element`. 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.
7. Specify the other alloying elements in the same way as you specify the first (for example, `c 1`).
8. 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.
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 in Step 6. For example, you can enter `Cr 5 Ni 1 Mo 0.5 C 0.01 N 0.02`.
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.
10. 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`.
11. 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`.
12. When prompted `OK?` type `N` to go back to Step 9 to reconsider which phases to reject or restore. Type `Y` to continue.

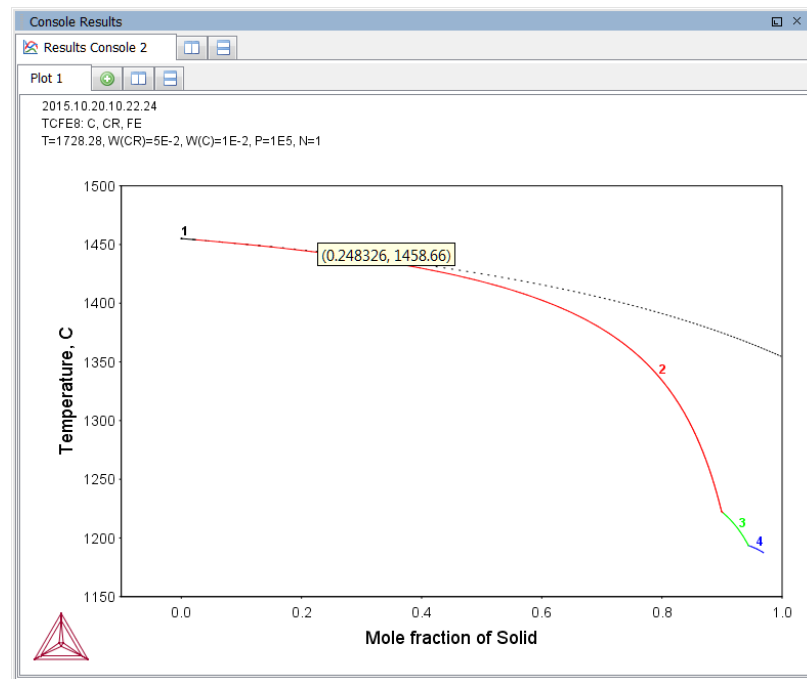
Thermodynamic data about the alloy system you defined is retrieved from the database.

13. At the Should any phase have a miscibility gap check prompt, press <Enter> for N or answer Y.

If you answer Y, you are prompted to specify the Phase with miscibility gap. Answer with a solution phase name(s) (in this example FCC is entered) as well as the Major constituents for sublattice (for each sublattice site) (for this example, Cr is entered for sublattice 1 and C for sublattice 2). In this example the Phase with miscibility gap is LIQUID PHASE NAME: LIQUID.

14. Press <Enter> to specify another phase.
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>. If you do specify any fast-diffusing components, then you are prompted to set whether BCC to FCC phase transformations should be simulated.

The Scheil-Gulliver solidification simulation runs, and the default diagram (Temperature versus Mole Fraction of Solid) is automatically plotted in the Console Results window.



10.3 Plotting Additional Scheil Simulation Diagrams

Post processing is done the same way as POLY-3 Post Processing module, specific variables for plotting in the Scheil Module are listed in the table.

The following 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.

Scheil State Variable Abbreviations

State variable	Abbreviation
Temperature in Celsius	T
Mole/mass fraction of liquid	NL/BL
Mole/mass fraction of all solid phases	NS/BS
Mole/mass fraction of a solid phase	NS(ph)/BS(ph)
Weight fraction of an element in a phase	W(ph,el)
Mole fraction of an element in a phase	X(ph,el)
Site fraction of an element in a phase	Y(ph,el)
Distribution of an element in a phases	NN(ph,el)
Heat release and Latent heat per mole/gram	NH/BH
Apparent heat capacity per mole/gram	CP/BCP
Molar volume of the system or a phase	NV/NV(ph)
Average density of the system or a phase	DS/DS(ph)
Apparent volumetric TEC of the system	BT

11. 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.


 Also see [Making a T0 Temperature Simulation](#) for step-by-step instructions.

11.1 Making a T0 Temperature Simulation

This section 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.

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_EQUILIBIRUM 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 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 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.



See Examples 23 and 41 in [Console Mode Examples](#).



Also see [Console Mode Visualisation](#).

12. 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.

 Also see [Calculating a Paraequilibrium](#) for step-by-step instructions.

 See Example 42 in [Console Mode Examples](#).

12.1 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 to set the conditions of your calculation just like when you calculate an ordinary equilibrium.
2. Use CHANGE_STATUS 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_EQULIBIRUM to run the calculation.
4. When you have calculated your initial equilibrium, use ADVANCED_OPTIONS then choose `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 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 then choose *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). The following figure is an example:


```

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 Example 23 in [Console Mode Examples](#).

13. Potential Diagrams

- [About Potential Diagrams](#)
- [Calculating a Potential Diagram](#)
- [Calculating a Potential Diagram with Different Pressure](#)

13.1 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 section describes how to calculate such potential diagrams with the POTENTIAL_DIAGRAM module (short name, 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.

13.2 Calculating a Potential Diagram

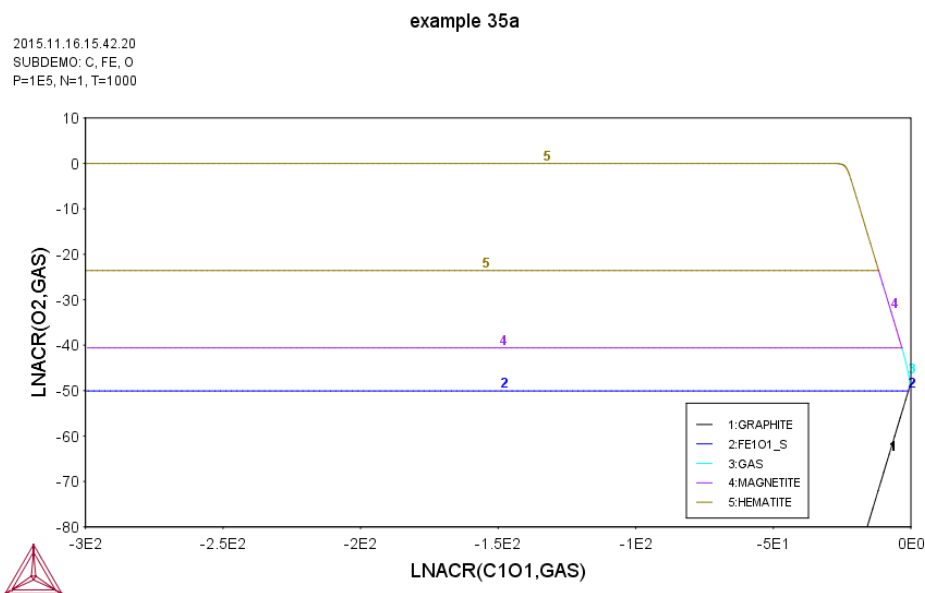
You need access to a substance or solution database that contains a gaseous mixture phase, metals (or alloys), and solids such as metal-oxides, sulphides, sulphates, carbonates, silicates, nitrides or nitrates (stoichiometric or solution phases). You can always use the TC Public Substances Database (PSUB), which is distributed with the Thermo-Calc program for free. It contains the six elements Fe, Cu, H, O, S and N.

1. Use GOTO_MODULE POTENTIAL to enter the POTENTIAL module.
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 your 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 from example 35 in [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.

13.3 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.

You must have calculated a potential diagram already, and have the saved POLY3-file available.

1. Use GOTO_MODULE POLY to enter the POLY module.
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.

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.

3. 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
```

4. 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.

5. Use MAP to perform the mapping calculations.
6. Use GOTO_MODULE POST to enter the POST module to set conditions for visualization and to plot the diagram.

14. Aqueous Solutions

- [About Aqueous Solutions](#)
- [Calculating a Pourbaix Diagram](#)
- [Plotting Additional Aqueous Solution Diagrams](#)
- [Stepping Calculations in an Aqueous Solution](#)
- [Pourbaix Examples TCEX40, 40A to 40E, and TCEX53](#)

14.1 About Aqueous Solutions

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 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.

You can calculate Pourbaix diagrams with the Pourbaix module. The compositional definition and variations and the basic solvent and electron components H_2O , $H+1$ and ZE are automatically determined by the aqueous solution phase in the Pourbaix module. These key components are defined as follows:

Component	Component status	Reference state	Ref-T(K)	Ref-P(Pa)
H_2O	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.

14.2 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.

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 H_2O , O_2 and H_2 . 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:

- `Reject phase(s) or Restore phase(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`

10. 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.

11. 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?)

14.3 Plotting Additional Aqueous Solution 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 following 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.

Aqueous Solution Variable Abbreviations

Variable	Abbreviation
Acidity	pH
Electronic Potential (V)	Eh
Electronic Affinity (kJ)	Ah
Electronic Activity (log10ACRe)	Pe
Ionic Strength	IS
Total Concentration	TM
Activity of Water	Aw
Osmotic Coefficient	Oc
Mole Fractions of Aqueous Species	MF(AQsp)
Molalities of Aqueous Species	ML(AQsp)
Activities of Aqueous Species	AI(AQsp)
Activity Coefficients of Aqueous Species	RC(AQsp)

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.

How to Plot an Aqueous Solution Diagram


1. Type **Y** 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:
 - change the axis-type (linear, logarithmic or inverse) on the X-axis or Y-axis
 - 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
 - refine the diagram in the POST Module
 - print the diagram (save a hard copy)
 - save the X-Y coordinates of curve on a text file
 - modify the plotted diagram
 - calculate and plot another aqueous solution diagram

14.4 Stepping Calculations in an Aqueous Solution

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.

 Performing the stepping calculation overwrites all the previous settings and stepping results on the POLY3-file. To avoid this, use **SAVE WORKSPACE** to create a new workspace.

You can use any of the following state variables as a stepping variable.

State variable	Abbreviation
Temperature (K)	T
Pressure (bar)	P
Acidity	pH
Electronic potential (V)	Eh

State variable	Abbreviation
Mole number of a dissolving component (such as Fe, Na, Cl, or NaCl) in 1 kg of water.	N(Comp) (for example, N (Fe))

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 $\log_{10}N$).

You must have plotted a Pourbaix diagram before making a stepping calculation on an aqueous solution.

Performing a Stepping Calculation

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.

14.5 Pourbaix Examples TCEX40, 40A to 40E, and TCEX53

TCEX40

- Using PAQ2 or PAQS2 database;
- For the Fe-H₂O-NaCl heterogeneous interaction systems
- With the Main Option 1
- Using the Single-Database Option, i.e., retrieving data from the PAQ2 [TCS Public Aqueous Solution (SIT) Database, v2.4; using the SIT aqueous solution model] or PAQS2 [TCS Public Aqueous Solution Database, v2.4; using the Complete Revised HKF aqueous solution model]; both of which contain 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 and PAQS2 are specially designed for

demonstrations of 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-PLOY-POST routine.

To further run the following Main Options:

Main Option 2 for plotting many other property diagrams of the calculated interaction system;

Main Option 3 for making another POURBAIX calculation of the same chemical system but under a different P-T-X condition;

Main Option 4 for making a POLY3 STEPPING calculation of the same chemical system but varied with only one independent variable;

** The Main Options 2, 3 and 4 are not illustrated in this TCEX40 example.

Five more examples (TCEX40A, TCEX40B, TCEX40C, TCEX40D and TCEX40E) are also provided to demonstrate various options and features in the POURBAIX module and to show more advanced applications of the TCAQ2 and AQS2 aqueous solution databases [in the Multiple-Database Option, i.e., with appended data from the SSOL5 and SSUB5 databases].

TCEX40A

- Option 1
- Using the Single-Database Option, i.e., retrieving data from the PAQ2 [TCS Public Aqueous Solution (SIT) Database, v2.4; using the SIT aqueous solution model] or PAQS2 [TCS Public Aqueous Solution Database, v2.4; using the Complete Revised HKF aqueous solution model]; both of which contain 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 and PAQS2 are specially designed for calculations of the so-called Pourbaix diagrams (i.e., Eh-pH plots) and other types of diagrams in aqueous-bearing multicomponent heterogeneous interaction systems, via the Single-Database Option in the POURBAIX module or through the normal TDB-GES-PLOY-POST routine.
- A POLY3 file called POURBAIX.POLY3 is automatically saved.
- For the purposes of recalling this file in other Main Options (as in the TCEX40B, TCEX40C & TCEX40D), the POURBAIX.POLY3 has to be renamed or copied as another file name (in this particular example, as TCEX40A.POLY3, and TCEX40B.POLY3, TCEX40C.POLY3 & TCEX40D.POLY3). Note that the renaming or copying has to be done outside TCCS, otherwise the POLY3 file structure will be destroyed. However, under WindowsNT/2000/XP environments, one can use MS-DOS commands to do so, e.g., @copy POURBAIX.POLY3 TCEX40B.POLY3
- The Main Option 1 also provides the opportunity to plot many property diagrams along phase boundaries, after the default Pourbaix diagram is generated and refined (not necessarily going through the Main Option 2).

TCEX40B

- Demonstration of the Main Option 2 Graphical Processing (by plotting more diagrams); various options for refining a plotted diagram (including direct interactions with the POST Module); Graphical processing of related property diagrams.
- Reading a previously saved POURBAIX.POLY3 file (or renamed as another name, for instance, the TCEX40B.POLY3), and then plotting some property diagrams for the previously calculated system.
- The loaded POLY3 file will not be modified by this Main Option. It is thus not necessary to save the file in another name; however, it is still recommended that the user to copy the TCEX40A.POLY3 (or TCEX40E.POLY3) as TCEX40B.POLY3 before the Main Option 2 is executed in this particular example.

TCEX40C

- Demonstration of the Main Option 3 Calculation (by modifying T-P-X conditions); graphical processing of a Pourbaix diagram.
- Reading a previously saved POURBAIX.POLY3 file (or renamed as another name, for instance, the TCEX40C.POLY3), and then making another POURBAIX-type calculation and graphical processing of a new Pourbaix diagram for the same chemical system but under a different P-T-X condition.
- The loaded POLY3 file will be rewritten according to the T-P-X settings in the new POURBAIX-type calculation. It is thus recommended to save the file in a new name outside of TCCS before this Main Option is proceeded (in this particular example, the TCEX40A.POLY3 is copied to TCEX40C.POLY3).
- The Main Option 3 also provides the opportunity to plot many property diagrams along phase boundaries, after the default Pourbaix diagram is generated and refined (not necessarily going through the Main Option 2).

TCEX40D

- Demonstration of the Main Option 4 Calculation (by utilizing various stepping variables); graphical processing of related property diagrams.
- Reading a previously saved POURBAIX.POLY3 file (or renamed as another name, for instance, the TCEX40D.POLY3), and then making some normal POLY3 STEPPING CALCULATIONS.
- The loaded POLY3 file will be rewritten according to the T-P-X and stepping variable settings in the stepping calculation. It is thus recommended to save the file in a new file name outside of TCCS before this Main Option is proceeded (in this particular example, the TCEX40A.POLY3 is copied to TCEX40D.POLY3).
- The resulting POLY3 file (in this example, TCEX40D.POLY3) can be subsequently called by a Main Option 2 for plotting more property diagrams, or by another Main Option 4 for making other stepping calculations.
- The Main Option 4 also provides the opportunity to plot many property diagrams after the default Pourbaix diagram is generated and refined (not necessarily going through the Main Option 2).

- Exploration of the possibility of modifying the definitions for some desired system-components, through the direct and internal POURBAIX-POLY3 intersection, for a STEPPING (and/or MAPPING) calculation inside the POURBAIX Module.

TCEX40E

- Demonstration of the Main Option 1 Calculation with the Multiple-Database Option; graphical processing of a Pourbaix diagram.

For a more complex application than in Example 40A.

This example requires licenses to three types of commercial Thermo-Calc databases otherwise it cannot be run, i.e.,

- A: TCAQ2 (TCS Aqueous Solution Database, v2.5; SIT model) or AQS2 (TGG Aqueous Solution Database, v2.5; HKF model);
- B: SSUB4 (SGTE Pure Substances Database, v4) or TCMP2 (TCS Materials Processing Database, v2);
- C: SSOL4 (SGTE Alloy Solutions Database, v4) or TCFE6 (TCS Steels/Fe-Alloys Database, v6) or ALIKE.
- This particular example uses the multiple-database combination of TCAQ2+SSUB4+SSOL4; among them, TCAQ2 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), SSUB4 database is appended for the Gaseous mixture phase and some pure solid phases (so-called secondary phases formed during aqueous-involving interaction processes), and SSOL database is also appended for various solid solution phases.
- A POLY3 file called POURBAIX.POLY3 is automatically saved. By reading this POURBAIX.POLY3 file (or renamed as another name), one can further run the following Main Options: Main Option 2 for plotting many other property diagrams of the calculated interaction system; Main Option 3 for making another POURBAIX calculation of the same chemical system but under a different P-T-X condition; Main Option 4 for making a POLY3 STEPPING calculation of the same chemical system but varied with only one independent variable; The Main Options 2, 3 and 4 are illustrated in the TCEX40B, TCEX40C and TCEX40D examples.
- For the purposes of recalling this file in other Main Options (as in the TCEX40B, TCEX40C & TCEX40D), the POURBAIX.POLY3 has to be renamed or copied as another file name (in this particular example, as TCEX40A.POLY3, and TCEX40B.POLY3, TCEX40C.POLY3 & TCEX40D.POLY3). Note that the renaming or copying has to be done outside TCCS, otherwise the POLY3 file structure will be destroyed. However, under Windows environments, one can use MS-DOS commands to do so, e.g., @copy POURBAIX.POLY3 TCEX40B.POLY3
- The Main Option 1 also provides the opportunity to plot many property diagrams along phase boundaries, after the default Pourbaix diagram is generated and refined (not necessarily going through the Main Option 2).
- The POURBAIX module inside the TCCS 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).

IMPORTANT NOTES FOR ACTIONS AFTER TCEX40A OR TCEX40E IS EXECUTED:

In order to be able to subsequently run the TCEX40B (Main Option 2), TCEX40C (Main Option 3) and TCEX40D (Main Option 4), which open the previously-saved POURBAIX-type calculation POLY3 file, the user should make four copies of the resulting POURBAIX.POLY3 as TCEX40A.POLY3, TCEX40B.POLY3, TCEX40C.POLY3 and TCEX40D.POLY3.

However, this has to be properly done outside of the TCCS software after the TCEX40A is executed. The reason is that, if saving the POLY3 workspace of the POURBAIX calculation results in the POLY3-module monitor (through the command sequence "GO PLOY3" and "SAVE TCEX40A.POLY3 Y"), all the initial equilibrium points and the mapping/stepping calculation results will be lost, and parts of the POLY3 file structure (e.g., some definitions of the previously defined POURBAIX-type calculation system) will be destroyed. In principle, before executing any Main Option (for calculations and graphical processing), it is highly recommended that the user shall save/rename/copy the previously-generated POLY3 file as another POLY3 file. Only in this way, it can avoid destroying the previous-saved POURBAIX-type calculation results.

Under Windows DOS-session (outside TCCS):

- copy POURBAIX.POLY3 TCEX40A.POLY3 (or TCEX40E.POLY3)
- copy POURBAIX.POLY3 TCEX40B.POLY3
- copy POURBAIX.POLY3 TCEX40C.POLY3
- copy POURBAIX.POLY3 TCEX40D.POLY3

or inside TCCS (under Windows NT/2000/XP, but not Windows 95/98/ME):

- @copy POURBAIX.POLY3 TCEX40A.POLY3 (or TCEX40E.POLY3)
- @copy POURBAIX.POLY3 TCEX40B.POLY3
- @copy POURBAIX.POLY3 TCEX40C.POLY3
- @copy POURBAIX.POLY3 TCEX40D.POLY3

Under Linux/UNIX platforms (outside TCCS):

- cp POURBAIX.poly3 TCEX40A.poly3 (or TCEX40E.poly3)
- cp POURBAIX.poly3 TCEX40B.poly3
- cp POURBAIX.poly3 TCEX40C.poly3
- cp POURBAIX.poly3 TCEX40D.poly3

TCEX53

- Using PAQ2 or PAQS2 database; for the Fe-X-H₂O-NaCl heterogeneous interaction systems (X = Cr-Ni-Co)

Note: The PAQ2 (TCS Public Aqueous Solution (SIT) Database, v2.4; using the SIT aqueous solution model) or PAQS2 (TCS Public Aqueous Solution Database, v2.4; using the Complete Revised HKF aqueous solution model) 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. Therefore, it can be used, via the Single-Database Option in the POURBAIX module or through the normal TDB-GES-PLOY-POST routine, for calculations of the so-called Pourbaix diagrams (i.e., pH-Eh plots) and other types of diagrams in aqueous-bearing multicomponent heterogeneous interaction systems.

Note: The initial bulk composition of Fe-based alloy in this demonstrating 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.

15. Tabulation of Chemical Substances, Phases or Reactions

The TAB module can be used to tabulate all kinds of 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.

 Also see [Tabulating a Reaction](#).

A reaction tabulation presents you with the following properties, on rows representing different temperature levels:

- Heat capacity change / Delta-Cp (Joule/K) in column 2.
- Enthalpy change / Delta-H (Joule) in column 3.
- Entropy change / Delta-S (Joule/K) in column 4.
- Gibbs energy change / Delta-G (Joule) in column 5.

Here is a screenshot of one such table:

```
*****
  T      Delta-Cp      Delta-H      Delta-S      Delta-G
  (K)    (Joule/K)    (Joule)    (Joule/K)    (Joule)
*****
```

T (K)	Delta-Cp (Joule/K)	Delta-H (Joule)	Delta-S (Joule/K)	Delta-G (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

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.

 Also see [Tabulating a Substance or Solution Phase at Fixed Composition](#).

You can add a 6th column to the table that shows the values of a property or user-defined function of your choice.

15.1 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.

15.2 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.

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 substances or 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.

16. Console Mode Visualisation

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).

- [Plotting Diagrams](#)
- [Modifying Diagrams](#)
- [Saving Diagrams](#)
- [Loading Saved Diagrams](#)

16.1 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 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 in POLY) and the Y-axis represents the sum of the mole fractions of all phases (that is, NP(*)).

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.

You use POST to enter the POST module (using GOTO_MODULE POST gives a NO SUCH MODULE message). The POST command is only available inside POLY.

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 to plot your diagram.

16.2 Modifying Diagrams

 Also see [Changing Global Settings](#).


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 to set diagram axis Y to $w(\text{Fe})$, and then use PLOT again to plot the new diagram.

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.

The following are some of the modifications you can make.

 Also see the *Thermo-Calc Console Mode Command Reference*.

- Use SET_TITLE 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 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.

 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

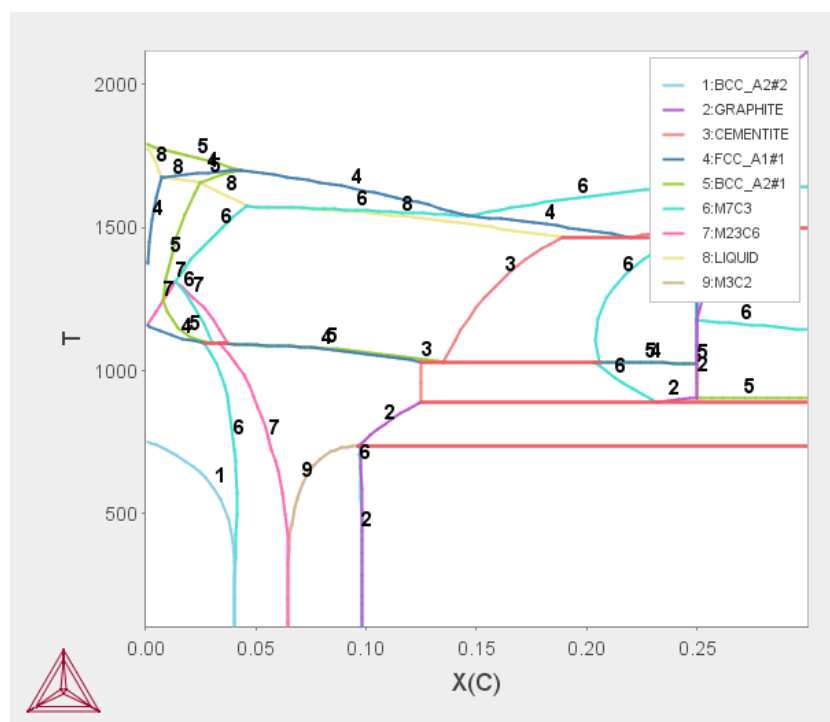
Symbol or text format	LTEXT	LaTeX
Subscripts in an axis text	S-A-TEXT Y N Mole-fraction Al ^{DO2} O ^{DO3}	S-A-TEXT Y N \latex Mole-fraction Al _{20_3}
Label with subscript	add .13 .15 n c-ZrO ^{DO2}	add .13 .15 n \latex c-ZrO ₂
Greek symbol	ADD .05 .50 N ^{GRd}	ADD .05 .50 N \latex \delta

- Use SET_AXIS_TYPE to set whether the scale of an axis is linear, logarithmic or inverse.
- Use SET_DIAGRAM_TYPE 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 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 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. The following screenshot shows how this might look:



16.3 Saving Diagrams

When a diagram is plotted, there are several ways in which you can save it:

- Use MAKE_EXPERIMENTAL_DATAFILE 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. For more information about DATAPLOT, search the online help or refer to the *DATAPLOT User Guide*.



Information about the underlying calculations that the diagram is based on is not saved in an EXP-file.

- Use DUMP_DIAGRAM to save the diagram image to a PS, PDF, SVG, EMF, GIF, or PNG file. You are asked what format to save it in.
- To save the diagram image in a variety of image file formats right click on diagram and choose **Save Plot**.
- Use PRINT_DIAGRAM to print a hard copy of the diagram.

16.4 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 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 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.

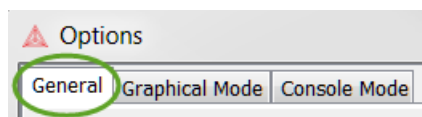
17. Changing Global Settings

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.



- [General](#)
- [Graphical Mode - Default Units](#)
- [Graphical Mode – Activities](#)
- [Graphical and Console Mode-Plotting](#)
- [Console Mode-Default Appearance](#)

17.1 General

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



General Global Settings

Setting	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 or Japanese .
Look and feel	To change the Look and feel of the GUI layout, choose Windows (the default), Metal , Nimbus , CDE/Motif or Windows Classic .
Database directory	<p>In the Database directory field, specify the path to the directory that contains the data directory. This is where the Thermo-Calc database directory is located. For example, the default for a Windows installation is:</p> <p>C:\Program Files\Thermo-Calc\<version>\</p> <p> Do not specify the path to where the database <i>files</i> are found (that is, in the data directory).</p> <p> Also see Modifying the Database Directory Path: Important Note.</p>
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.

Setting	Options
Check update interval	From the Check update interval list, choose not to check (Don't check , the default) or On startup . You can also manually check for updates – choose Help → Check for update .
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.

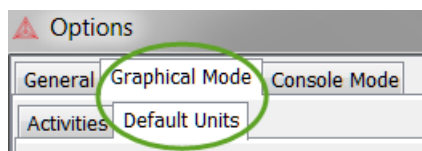
Modifying the Database Directory Path: Important Note

Any licensed databases purchased from Thermo-Calc Software are encrypted in files with the extension .tdc; these files cannot be edited. Unencrypted databases have the file extension .tdb. For example, user-defined database files can be modified.

All databases located in the database directory path are cached after they have been read once to ensure that the standard databases included with Thermo-Calc are loaded quickly and efficiently into the program. 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.

17.2 Graphical Mode - Default Units

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



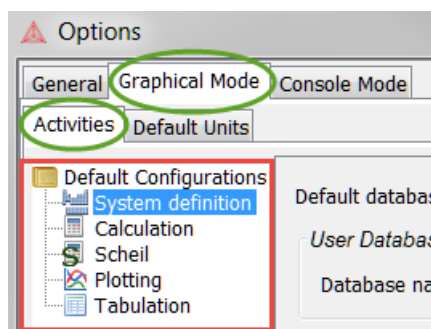
Default Units - Settings in Graphical Mode

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

Setting	Options
Time	Seconds (the default), Hours or Days
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.

17.3 Graphical Mode – Activities

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



There are **System definition**, **Calculation**, **Scheil**, **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).



Also see [Graphical and Console Mode-Plotting](#).

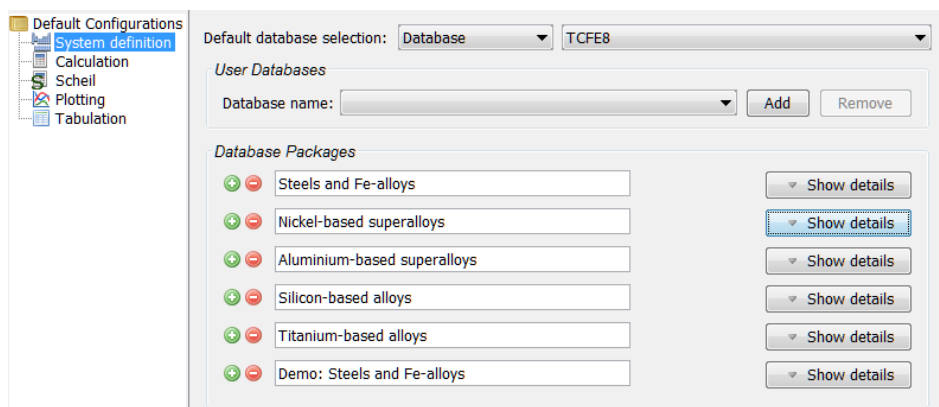
17.3.1 System Definition (System Definer)

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**.





Also see [System Definer](#).



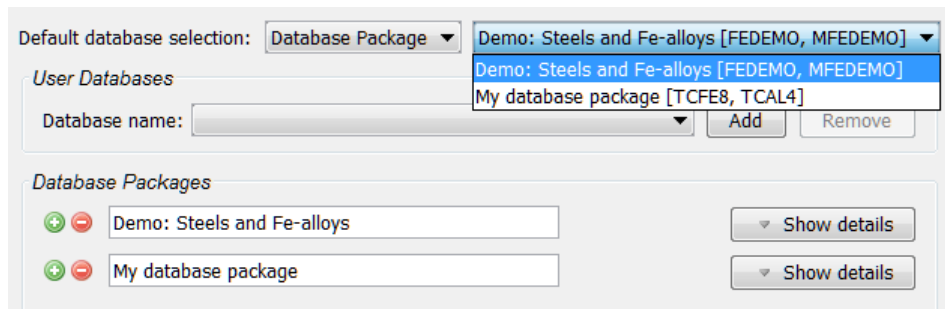
System Definer Default Settings in Graphical Mode


Setting	Options
Default database selection	<p>Choose to define a Database or a Database package.</p> <p>If you choose Database, then select the default installed database to use globally for all System Definer nodes. For example, choose TCFE8 or TCNI8.</p> <p>If you choose Database Package, select an option from the list. These Database Packages are defined in the section <i>Database Packages</i>.</p>
<i>User Databases</i>	
Database name	<p>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.</p> <p>Once a user database is added to the Database name list, you can also click the Remove button to delete it from your project.</p>
<i>Database Packages</i>	
Based on the installed databases, there are also default Database Packages available.	<p>Create and remove Database Packages by clicking the Add a database package  button or Remove this database package  button.</p> <p> The addition or removal of a database package does not take effect until a new System Definer node is defined.</p> <p>Click Show details to display the list of databases included with the package. Click Hide details to only display the name of the package.</p> <p> Also see Creating a Database Package.</p>
Reset to original settings	<p>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.</p>

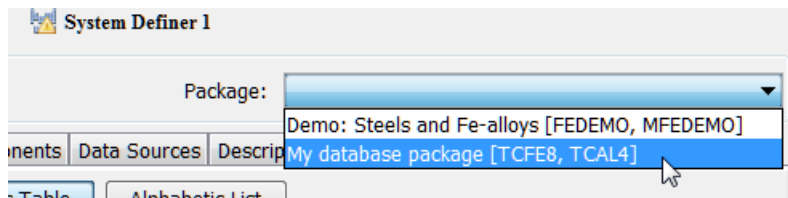
Creating a Database Package

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, **TCNI8**.
6. Click the **Add a database**  button and from the **Choose database** list, select another database, for example, **TCAL4**.

- Click **OK**. The Database Package is now available to choose as the default for new System Definer activities.



-  The package is available for new [System Definer](#) nodes defined after adding the package.

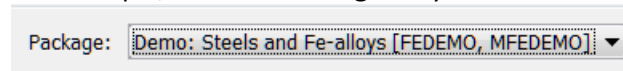


Clearing a Database Package Message

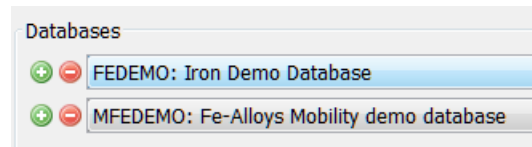
Sometimes when working on the [System Definer](#) Configuration window, you may add or delete Databases. If you originally added a Database Package, the addition or removal of a database means that the original package you selected does not now match the databases you are using. To clear the message *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.

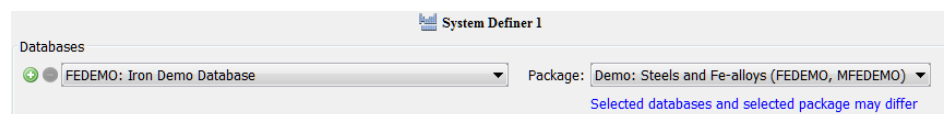
For example, from the **Package** list you select **Demo: Steels and Fe-alloys**.




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.

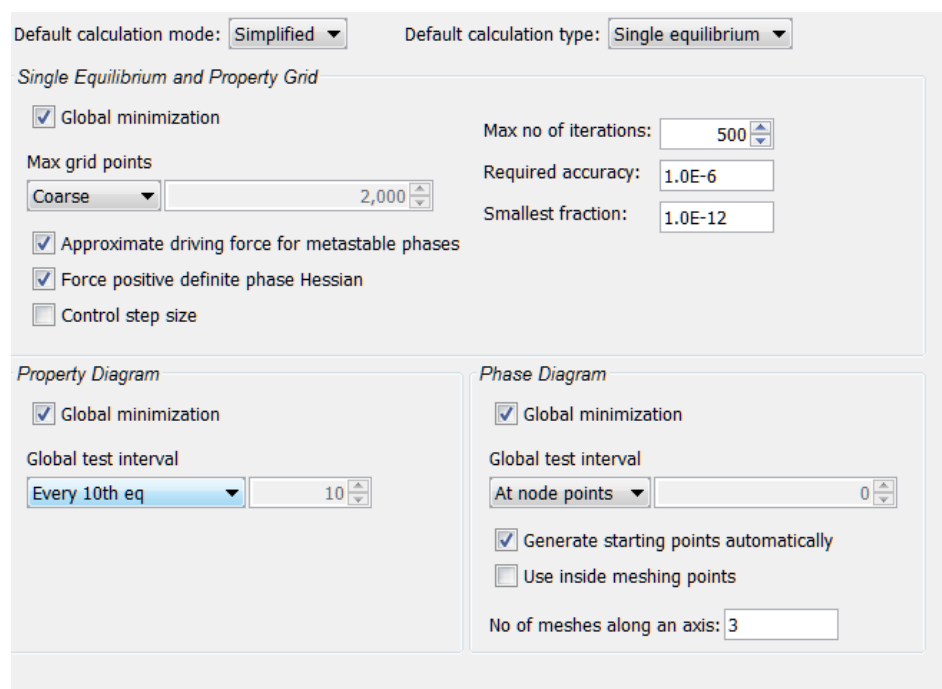
17.3.2 Calculation (Equilibrium Calculator)

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**.

 Also see [Equilibrium Calculator](#).

These settings can also be changed locally for a certain Equilibrium Calculator.



Equilibrium Calculator Default Settings in Graphical Mode

Setting	Options
Default calculation mode	Simplified (the default) or Advanced
Default calculation type	Single equilibrium (the default), Property diagram, Phase diagram or Property grid
<i>Single equilibrium and property grid</i>	
Global minimization	The check box is selected by default to ensure that the most stable minimum under the specified conditions is computed.
Max no of iterations	Default is 500
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)

Setting	Options
Required accuracy	The default is 1.0E-6
Smallest fraction	The default is 1.0E-12
Approximate driving force for metastable phases	The check box is selected by default
Force positive definite phase Hessian	The check box is selected by default
Control stepsize	The check box is selected by default
<i>Property diagram</i>	
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	Every 10 th eq (the default), Always or Custom
<i>Phase diagram</i>	
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 10 th eq, Always or Custom
Generate starting points automatically	The check box is selected by default
Use inside meshing points	Click to select the check box as required
No of meshes along an axis	The default is 3
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.

17.3.3 Scheil (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**.

 Also see [Scheil Calculator](#).

These settings can also be changed locally for a certain Scheil Calculator.

Scheil Calculator Default Settings in Graphical Mode

Setting	Options
Start temperature	Enter a default 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 default Temperature step . Decreasing the temperature step increases the accuracy, but the default value is usually adequate.
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.
Allow BCC → FCC	By default the Allow BCC → FCC check box is not selected. Select the check box to allow transformations in the solidified part of the alloy caused by each of the components specified to be a <i>fast diffuser</i> . It is recommended that you only select this for steels.
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.

17.3.4 Tabulation (Table Renderer)


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**.

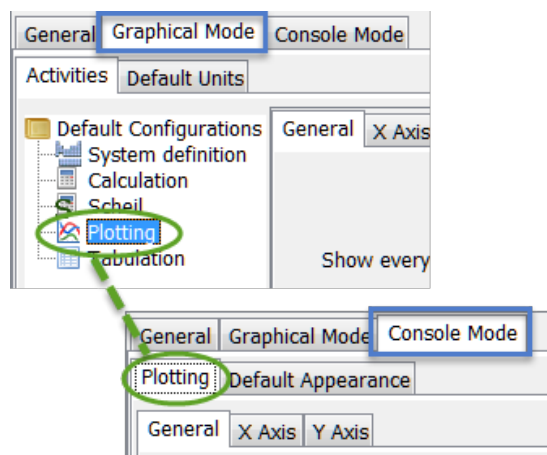
 Also see [Table Renderer](#).

Table Renderer Default Settings in Graphical Mode

Setting	Options
Decimal digits	The default is 5
Number format	Auto (the default), Decimal or Scientific
Phase description detail	Composition (the default), Condensed, Constitution, or Composition and constitution
Primary display color	Click Modify to change the default
Secondary display color	Click Modify to change the default
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.

17.4 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).



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.

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 Ctrl while you move the cursor around the plot to only display it as a crosshair and prevent unintended edits.



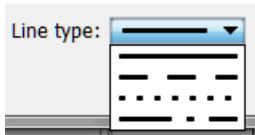
To globally configure the default settings for plotting, from the main menu select **Tools** → **Options**. Click the **Graphical Mode** → **Activities** tabs and then click the **Plotting** node.

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.

Plot Renderer Settings for Console and Graphical Modes

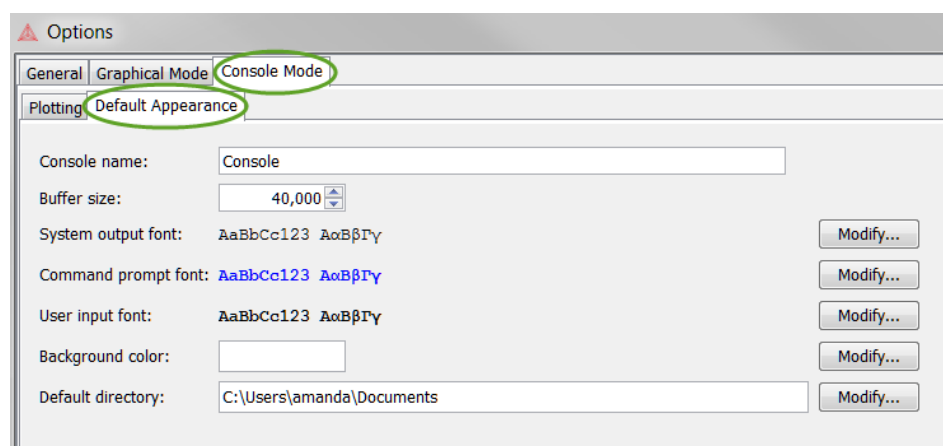
Setting	Options
Title	<p>Enter a title. Select Plain text (the default) or LaTeX formatted text.</p> <p>Click α button to add symbols. Click a symbol category (for example, Latin characters or Greek and math symbols). Then click to choose the symbol located on the right-hand side.</p>

Setting	Options
	<p>When you select LaTeX formatted text you can use the LaTeX math text to enter text.</p> <p> For a list of supported LaTeX commands, see http://www2.ph.ed.ac.uk/snuggletex/documentation/math-mode.html</p>
Title font, Legend font, Label font, Header font	Click Modify to edit the Font Name, Style, Size and Color.
Legend phase caption style	<p>Choose All, Constitution description or Ordering description.</p> <p> Also see About Legend Styles.</p>
Legend background color, Background color, Canvas color, Border color,	Click Modify to choose a color or enter a specific color.
Label format	Select Plain text (the default) or LaTeX formatted text.
Show anchor	By default, an anchor between the label and the plot point is displayed.
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.
Border width	Choose a plot border width between 1 (thin, the default) and 10 (thick).
Color option	<p>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.</p> <p>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.</p>
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	<p>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.</p> <p></p>


Setting	Options
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 point marker size	Choose the data point marker size between 1 (small) and 10 (large). The default is 3.
Plot Area Size	The Fit the plot area size to the enclosing window option is selected by default. Excluding triangular plots, click Define the plot area size to enter a Plot area height and Plot area width.
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.

17.5 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**.



Default Appearance Settings in Console Mode

Setting	Options
Console name	The default is <code>Console</code> or enter another name to display
Buffer size	The default buffer size is 40,000.  Also see Increasing the Buffer Size .
System output 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	
User input font	
Background color	Click Modify to open the Select Color window to choose a background color for the Console Mode window where you enter commands.

Setting	Options
Default directory	Set the default directory where log files and workspace files 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.

17.5.1 Increasing the Buffer Size

Sometimes the output overflows the window text buffer.

 Also see [Controlling Console Output](#).

To increase the buffer size in a specific Console tab:

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

