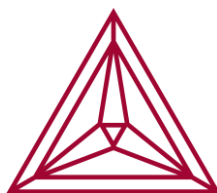


**Thermo-Calc
Software**

Thermo-Calc Console Mode User Guide

Version 4.1



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Thermo-Calc Console Mode User Guide

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1 Introduction

1.1 The Thermo-Calc software package

Thermo-Calc is a sophisticated software, database and programming-interface package for performing thermodynamic calculations. It allows you to calculate complex homogeneous and heterogeneous phase equilibria, and plot the results as property diagrams and phase diagrams.

The program 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 can take into account wide ranges of temperature, pressure and compositions conditions.

A Software Development Kit (SDK) is available for the Thermo-Calc program. This SDK can be used to plug the Thermo-Calc calculation engine into your own applications or into various third-party applications.

There are two interfaces to the Thermo-Calc program, the Console Mode which uses a command line interface and the Graphical Mode which has a graphical user interface (GUI). This User Guide describes the use of the Thermo-Calc program in the Console Mode.

The Thermo-Calc program also includes modules for running simulations of diffusion controlled transformations in multicomponent systems, DICTRA and DIC_PARROT. For information about how to use this DICTRA part of the Thermo-Calc, see the *DICTRA User Guide*. Note that in order to use these modules, you need a separate DICTRA license.

1.2 Documentation for Thermo-Calc Console Mode

Apart from this document, you can use the following documentation to learn more about how to use Thermo-Calc in the Console Mode:

Thermo-Calc Console Mode Command Reference

contains information about all the commands that are available in the Thermo-Calc Console. For each command there is a brief description of what the command does, what the command's parameters are (if any), and what kind of values you can give the parameters

Online help in the Thermo-Calc Console Mode

contains information about modules, commands, and conditions

Thermo-Calc Console Examples Collection

contains over fifty example macro files that demonstrate different ways in which you can use Thermo-Calc. See Appendix 2 – List of examples in the Thermo-Calc Console Examples Collection.

DATAPLOT User's Guide and Examples

describes the syntax and semantics of the DATAPLOT graphical language, which is used to store information about thermodynamic diagrams

Data Optimisation User Guide for Thermo-Calc

describes how to use perform data optimisations in Thermo-Calc using the PARROT module.

DICTRA Module User Guide

describes how to use the DICTRA_MONITOR module in Thermo-Calc. Note that in order to use DICTRA, you need a valid DICTRA license.

Additional documentation and educational materials are available on Thermo-Calc Software's website.

1.2.1 This User Guide

Target group

This user guide is intended for new users of the Thermo-Calc console mode that are not familiar with the command-line interface. It is expected, however, that such a user does understand the basics of thermodynamics.

Purpose

This Thermo-Calc Console Mode User Guide is intended to get you started using Thermo-Calc in the Console Mode. It gives you a brief overview of the program and its various components, describes how the command line user interface works, and describes how, in generic terms, you can define your system of components, set up calculations, perform calculations and visualize the results.

Content

After this Introduction chapter, chapter 1.4 describes how you use the Thermo-Calc Console Mode interface. The chapters that then follow each describe a step in the typical Thermo-Calc workflow. Chapter 0 describes how you define which elements your system contains and retrieve necessary thermodynamic data about these elements. Chapter 4 describes how you set up and perform various kinds of calculations, and plot the results as property or phase diagrams of various kinds. Finally, chapter 0 describes how you can modify how a diagram is plotted, change the appearance of your diagram, and save it in different formats. There are also three appendices that provide additional information that may be useful when you are using Thermo-Calc. Some of this information will only be of interest once you have become a more advanced user of the program.

Note that this User Guide only scratches the surface of what you can do with Thermo-Calc. Thermo-Calc is a very powerful and flexible program. At every stage in the workflow, there are a host of different parameters and conditions that you can modify to tweak and tune your material system, the calculation, or the visualization of the results. Once you have learned the basics from this User Guide, you can turn to other learning resources.

Thermo-Calc can be used in two interface modes: the Console Mode and the Graphical Mode. This guide only describes how you use Thermo-Calc in the Console Mode. For information about how to use Thermo-Calc in the Graphical Mode, see the *Thermo-Calc Graphical Mode User Guide*.

The following conventions will be used:

- Console command name are written in small upper case letters. For example, the command for calculating an equilibrium is `COMPUTE_EQUILIBRIUM`.
- Examples of how you can use a command are written like this:

```
SET_CONDITION T=1000 P=1E5 X(C)=0.01 N=1
```
- Menu items are referred to by the menu name and the name of the item, separated by a vertical line ("|"). For example, "select Tools | Options" means, select the menu item "Options" from the Tools main menu.

1.2.2 Using online help

At the command line prompt in the Console, you can access online help information in several ways:

- To get a list of all the available commands in the current module, simply type a question mark ("?",) and press the enter key.
- To get a description of a specific command, use `HELP` followed by the name of the command. Note that you can only get online help information about a command that is available in the module that you are currently in.
- To get more general information about the system, use `INFORMATION`. You will be requested to specify about which subject you want information. Answer "?" in response and you will get a list of all the subjects on which you can get more information. Note that this subject list is specific to the module you are currently in.
- To access some online help that you can read in a web browser, select "Help | Help Contents". From this help contents, it is also possible to access some documentation available as PDF-files, including this User Guide.

1.2.3 Contents of the Thermo-Calc Console Examples Collection

To learn more about how to use Thermo-Calc, you can run and study the examples in the *Thermo-Calc Console Examples Collection*. This is a collection of extensively commented macro files that 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 will not see the output that Thermo-Calc gives in response to the commands stored in the macro file. However, the pdf document *Thermo-Calc Examples* also shows the output for each example.

A table provides a brief description of each example in Appendix 2 – List of examples in the Thermo-Calc Console Examples Collection.

1.3 Program overview

The Thermo-Calc program consists of several basic modules that handle database retrieval and management, calculation and optimisation, and visualization and diagram plotting.

Most modules are managed using commands but some modules, called response-driven modules, prompt you with a series of questions which typically take you through the whole process of defining your system, setting conditions on the calculation, performing the calculation and plotting the results.

1.3.1 Modules

The following table lists and briefly describes Thermo-Calc's various modules:

Abbr. Name	Full Name	Primary Functions
BIN	BINARY_DIAGRAM	This response-driven module lets you calculate binary phase diagrams. To use this module, you need access to databases that were designed for the BIN module, such as the TCBIN database.
DATA	DATABASE_RETRIEVAL	The DATA module lets you select appropriate database, define your chemical system and retrieve the data required for your calculation.
DICTRA	DICTRA_MONITOR	The DICTRA module lets you run simulations of diffusion controlled transformations in Thermo-Calc. Note that if you do not have a DICTRA license, then you cannot enter this module. See the <i>DICTRA User Guide</i> for more information.
DIC_PARROT	DIC_PARROT	This is the data optimisation module for DICTRA. It allows you to assess experimental data and use such data to optimise calculations. Note that if you do not have a DICTRA license, then you cannot enter this module.
ED_EXP	EDIT_EXPERIMENTS (PARROT submodule)	ED-EXP is a submodule that is part of PARROT. It allows you to edit experimental data points in order to make reliable optimisations.
GIBBS	GIBBS_ENERGY_SYSTEM	The GIBBS module handles thermodynamic models and thermodynamic quantities. Typically, you will not be directly interacting with this module, but if you do, you can get information about models, and list, add or amend the thermodynamic parameters being used.

Abbr. Name	Full Name	Primary Functions
PARROT	PARROT	This data optimisation module lets you assess experimental data and use such data to optimise calculations. See the <i>Data Optimisation User Guide for Thermo-Calc</i> for more information.
POLY	POLY	The POLY module is the equilibrium calculation module. This is module in which you will specify conditions for calculations and perform those calculations.
POST	POST_PROCESSOR (POLY submodule)	POST is a submodule that is part of POLY. It handles all the post-processing and plotting of calculation results. In this module you can modify the property and phase diagrams, add labels, change the colours used in the diagrams, etc.
POTENTIAL	POTENTIAL_DIAGRAM	This response-driven module lets you calculate and plot gas potential diagrams in a ternary system. The potential of two gas species are used as the diagram axes.
POURBAIX	POURBAIX_DIAGRAM	This response-driven module calculates and plots pH-Eh diagrams, also called Pourbaix diagrams) and various property diagrams for heterogeneous interaction systems involving aqueous solutions.
REACTOR	REACTOR	This module lets you simulate chemical reaction processes in several feed-forward steady-state stages or in several dynamic stages.
SCHEIL	SCHEIL_SIMULATION	This response-driven module lets you 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).

Abbr. Name	Full Name	Primary Functions
SYS	SYSTEM_UTILITIES	This is the module that is opened when you start up Thermo-Calc. The SYS module lets you interact with your operating system and change environmental settings. It also enables you to create and execute MACRO files.
TAB	TABULATION	This module allows you to tabulate various properties of chemical reactions and substances (stoichiometric or solution phases).
TERN	TERNARY_DIAGRAM	This response-driven module lets you calculate ternary phase diagrams.

1.4 Licenses for using Thermo-Calc

To use Thermo-Calc, you need a valid standalone “LSERVRC” license file (of you have a standalone installation of Thermo-Calc) or access to license server with a valid network “LSERVRC” license file (if you have a network client installation). If you start Thermo-Calc without a valid Thermo-Calc license, then you will not be able to do any calculations and you will not be able to leave the SYS module.

Note that if you are using a network client installation of Thermo-Calc, then you may not be able to enter the POLY module even if you have access to a license server with a valid network license file. This is because other clients that are part of your network installation may have “checked out” all instances of Thermo-Calc that the network license allows you to run simultaneously. For more information, see section 2.6.

To be able to enter the DICTRA and the DIC_PARROT modules, you also need a valid DICTRA license key. As in the case of Thermo-Calc, if you are running DICTRA on a network installation, it is possible that you cannot enter the DICTRA module because all the instances of DICTRA that the network license allows you to run simultaneously have been checked out.

Note also that if you enter and use either the DIC_PARROT module or the PARROT module, then you will not be able to 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. If you try to enter PARROT after having been in the DIC_PARROT module, then you will get the following message:

```
PARROT disabled after using DICTRA PARROT
```

For more information about the DICTRA module, see the *DICTRA Module User Guide*.

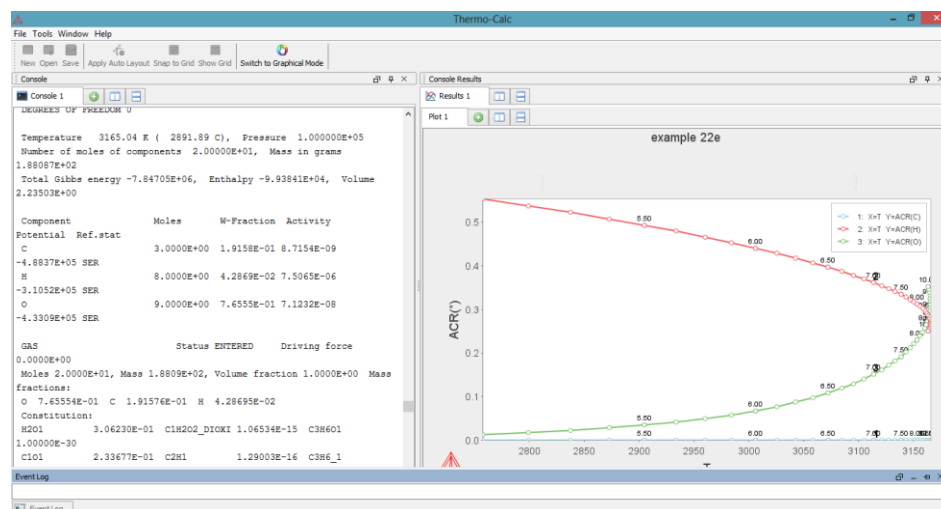
2 Using the console interface

This section briefly introduces you to the Console Mode's user interface and the command line prompt. You can also read about how to save your work in Thermo-Calc. The basic workflow of the program is also described.

2.1 The Thermo-Calc Console Mode interface

When you open Thermo-Calc, the program will by default be opened in the Graphical Mode. To enter Console Mode, click »Switch to Console Mode» on the toolbar.

The following screen shot shows the Thermo-Calc Console Mode user interface:




There are three windows: the “Console” window, the “Console Results” window, and the “Event Log” window.

The window that you are currently working with or have selected is called the “active” window. This window has darker window title bar than the other two windows. (In the preceding screenshot, the empty “Event Log” at the bottom of the screen is the active window.)

“Console”

This window is by default placed on the left side of the screen. This is where you type your commands. The Console window may contain several Console tabs.


There are several ways of opening and closing additional Console tabs:

- To open a Console tab, click the «Add button» , press Ctrl+T when the Console window is active, or right-click a tab header and select “New Console” from the pop-up menu.
- To close a Console, click the small «Close button» (the “x” on a tab’s header), press “Ctrl+W” or “Ctrl+F4”, or right-click the tab header and select “Close” from the pop-up menu.

- To close all tabs except one, right-click the header of the tab you want to keep and select “Close Other” from the pop-up menu.
- To close all Console tabs and open a new clean one, right-click the header of any tab and select “Close All” from the pop-up menu.

You can change the tab name, font and colours for an individual Console tab by right-click its header and selecting “Properties” from the pop-up menu.

“Console Results”

This window is by default placed on the right side of the screen. This is where diagrams that are plotted will appear. Each Console has its own Results tab in the Console Results window. All the plots and tables generated from the console will be presented in that Results tab. You can open new additional Plot tabs by pressing “Ctrl+Shift+T” or by clicking the «Add button» .

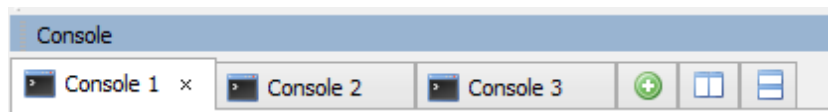
You can also open and close additional Plot tabs when you are working in a Console tab (that is, when the Console window is active). To open a new Plot tab for the currently active Console tab, press “Ctrl+Shift+T”. To close the Plot tab that is currently shown on the Results tab, press “Ctrl+Shift+W” or “Ctrl+Shift+F4”.

“Event Log”



This window is opened by you and displays information about the commands that run and are completed, including any error messages..

If you close any of these windows, you can open them again by selecting the “Console”, “Console Results” or “Event Log” item on the “Windows” menu. To realign the windows to the original layout, select Windows | Reset Windows.

By default, different tabs are presented as one on top of each other in the following way:



To view as certain tab, simply click on the header of that tab. You can also view tabs laid out side-by-side or top-to-bottom in both the Console and the Console Results window. Do this by clicking the «Show tabs side by side

button»  or the «Show tabs stacked button» . To return to showing the tabs on top of each other as in the preceding screen shot, click the «Tab

label button» .

2.2 Working with tabs in the Console window

In the Console window, there are more ways in which

2.3 Using the command line prompt

The command line prompt in the Console window tells you which module you are currently in. When you open Thermo-Calc in the Console Mode, you will find yourself in the SYS module, and this is indicated by the fact that the command line prompt is "SYS:"

To use Thermo-Calc in the Console Mode, you type in commands at the command line prompt. Which commands are available to you depends on which module you are in. To see a list of all the commands that are available in the module you are in, type "?" and press the enter-key.

2.3.1 Command names and abbreviations

The name of a command typically consists of several terms linked by underscore characters, such as LIST_EQUILIBRIUM. It does not matter whether you type in commands in upper or lower case letters.

You can abbreviate all Thermo-Calc commands as long as the abbreviation is unambiguous. Each word in the command name can be abbreviated separately. For example, LIST_EQUILIBRIUM can be abbreviated L_E. Instead of the underscore character, you can separate the words in a command name by a hyphen ("-").

The following table shows examples of how you can abbreviate some command names:

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
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

2.3.2 Specifying parameters

Running a command typically requires that a number of parameter values be specified. Parameters can be specified directly at the command line after the command name. For example, to set an axis variable for a stepping or mapping operation, you could directly enter:

```
SET_AXIS_VARIABLE 1 X(FCC,FE) 0 0.89 0.025
```

Alternatively, you could type SET_AXIS_VARIABLE and simply press the enter key. At the command line prompt, you would then be requested to specify the parameters one by one.

If you are not sure what your alternatives are, or what the requested parameter is, then you can try answering with a question mark ("?"). Typically, a brief explanation will then follow. For some parameters, more detailed information will be presented if you answer with two question marks ("??").

2.3.3 Default parameters values

When you are requested to specify a parameter, Thermo-Calc usually suggests an appropriate default value or answer. Such a default value or answer is given between two slash signs ("/") at the prompt. For example, the following prompt indicates that the default answer is "terminal":

```
OUTPUT FILE /TERMINAL/:
```

To accept the default value or answer, simply press the enter key.

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 (",,,") will be interpreted in the same way as " , , , ").

For some commands and parameters, Thermo-Calc treats the values that you have previously assigned to them as default values if the command is used again. For example, suppose that the first stepping or mapping axis variable is specified in the following way:

```
SET_AXIS_VARIABLE 1 X(FCC,FE) 0 0.89 0.025
```

If you later want to change one parameter value for this axis variable, then you could type:

```
SET_AXIS_VARIABLE 1 , 0.1 , , ,
```

This will change the minimum value from 0 to 0.1 at which a stepping or mapping operation will halt. The other parameter values will remain the same. Consequently, what you typed in would be equivalent to the following:

```
SET_AXIS_VARIABLE 1 X(FCC,FE) 0.1 0.89 0.025
```

2.3.4 Controlling Console output

Thermo-Calc may print a lot of text in the Console window in response to a command. You can pause the printing of the output by pressing “Ctrl-S”. To resume the printing on screen, press “Ctrl-Q”.

Occasionally, the output to screen can overflow the text buffer of the window. If this happens, then it may be useful to increase the buffer size of the current Console tab.

How to increase the buffer size

To increase the buffer size in a certain Console tab, perform the following two steps:

Step	Action
1	Right-click on the Console tab header in the Console window (if this is the first Console tab, it will be labelled “Console 1”)
2	Click on “Properties”, and then increase the “Buffer size” in the Console Properties window.

Note that this only changes the buffer size of the particular tab whose header you right-clicked. To change the buffer size of any new tabs that you will create, select Tools | Options, then select the “Console Mode” tab where you can increase the default “Buffer size”.

When Thermo-Calc is performing a mapping operation, the results will be continuously printed in the Console window. To terminate the calculation of the current region of the mapping and stop the output, press “Ctrl-C”.

2.3.5 Command history

To scroll through the last twenty commands that you have used, type two exclamation marks (“!!”) and press the enter key. To repeat the last n commands, type “!” followed by the number of previous commands that should be executed again. To scroll through previous performed commands, use the Up or Down arrow keys (“↑” or “↓”).

To read more information about the command history functionality in Thermo-Calc, type “! ?” at the command line prompt.

2.3.6 Wild card characters

You can sometimes use the asterisk (“*”) as a wild card character to, for example, refer to all components, all phases, or all species. For instance, you can do this 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. The asterix and the dollar sign normally does not work properly as wild card characters for referring to activity and/or chemical potential properties.

The following table shows ways in which you can use these wild card characters.

Command	Action
SHOW_VALUE B(*)	Lists mass (gram) of all components in the system.

SET_AXIS_VAR Y B(*) *	Sets mass (gram) of all components in the system as Y-axis variable.
SHOW_VALUE MUR(*)	Lists chemical potentials of all components in the system.
SET_AXIS_VAR Y ACR(*) *	Sets activities of all components in the system as Y-axis variable.
SHOW_VALUE HM(*).T	Lists heat capacities of all phases.
SET_AXIS_VAR Y GM(*) *	Sets molar Gibbs free energies of all phases as Y-axis variable.
SHOW_VALUE TC(\$)	Lists curie temperature of all stable phases.
SHOW_VALUE W(*,*)	Lists mass fractions of all components in all phases.
SHOW_VALUE W(\$,*)	Lists mass fractions of all components in all stable phases.
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.

2.4 Using log, macro, and workspace files

In the console mode, Thermo-Calc makes use of a few different kinds of files, including log files (*.LOG), macro files (*.TCM or *.LOG), POLY workspace files (*.POLY3), and experimental data files (*.EXP). The GIBBS module makes use of its own type of workspace files (*.GES5), and the PARROT module makes use of files with the suffixes *.PAR and *.POP. When you start using Thermo-Calc in the console mode you will mainly make use of log files, macro files and POLY workspace files.

For information about experimental data files, see the *DATAPLOT User Guide* and the *Data Optimisation User Guide for Thermo-Calc*.

2.4.1 Using 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 Thermo-Calc's output in the log file as well, use `SET_ECHO` before the `SET_LOG_FILE` command. Doing this is often useful if you want use the log file later as a macro file.

2.4.2 Using 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. To load a macro file, use `MACRO_FILE_OPEN` in the `SYS` module, followed by the name of the macro file. Thermo-Calc will then immediately execute the command sequence that the file contains.

If you end a macro file with the `SET_INTERACTIVE` command, then control of the Console will be given back to the user.

You can make a macro file load other macro files inside it by adding a `MACRO_FILE_OPEN` command when creating the log file that you want to use as a macro file. You can in this way have at most five nested levels of macro files. If a nested macro file ends with `SET_INTERACTIVE`, then Thermo-Calc will resume with the higher-level macro file at the command immediately following after 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 will shut down and the macro will be aborted.

You add comments to a macro file by starting a line with "`@@"`", or by enclosing them between a "`@(-`"-line and a "`@)`"-line. All lines in the macro file that are between these lines will be ignored by Thermo-Calc when you are running the macro.

Control characters

The "`@?`" character allows you to make a macro interactive by allowing input from the user. At the "`@?`" character, which should be placed where a parameter value or argument would normally be put, Thermo-Calc will prompt the user to input the value of a parameter or argument. You can enter a string immediately following the "`@?`"-character. This string will be presented to the user when prompted to enter the parameter value or argument. The entered value will be 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 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 could write:

```
SET_AXIS_VARIABLE 1 x(##3) 0 1,,,
```

Finally, there is the “@&” pause character. Thermo-Calc pauses and waits for input from the user when this pause character is read from a macro file. Inserting pause characters is useful if you want to allow the user to monitor what is happening when Thermo-Calc is running the macro.

Response-driven modules and macros

Macro files that are created while you use a response-driven module begin with the module-entering command (for example, `GOTO_MODULE SCHEIL`) followed by a number of lines with responses to the module’s questions and requests. The file terminates with the `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).

2.4.3 Using workspace files

You can save all the data in your current workspace by first using `SAVE_WORKSPACES`. This command is available in the `POLY` module, as well as in the `GIBBS` and `PARROT` modules. The workspace will contain all the settings you have specified and the result of any stepping or mapping operations that you have 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 has been executed. The saved data will include original and modified thermodynamic data, your last set of conditions and options, and the results of any calculations.

To load the data and calculation results of a workspace file, use the `READ_WORKSPACES` command that is 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.

When you go to a response-driven module such as `POTENTIAL` or `SCHEIL` for example, a workspace file will automatically be opened. In the workspace file, system definitions, conditions for the calculation, calculation results, and plot settings will be saved. The file will be saved in the current working directory, and will be named after the name of the module that created it. For example, the `POTENTIAL` module will save a workspace file called `POT.POLY3` (or `POT.poly3` in Linux); the `POURBAIX` module will save a file called `POURBAIX.POLY3`; etc.

2.5 Default options

You can set general settings for Thermo-Calc Console mode in the “Options” window. To open this window, select “Options” from the “Tools” main menu. The tabs and panes that are relevant for Thermo-Calc Console mode are briefly described in the table that follows:

Tab / pane	Description
------------	-------------

General	<p>Here you can select whether to turn on tooltips information. If “Tooltips enabled” is selected, then a small text box will appear when you hold the cursor still above some buttons or other items.</p> <p>Here you can also select which language that will be used in the program, and change the appearance of the program (“Look and feel”).</p> <p>In the “Database directory” field, specify in which directory the Thermo-Calc database directory called “data” can be found. Note that you are not supposed to specify the path to where the database files can be found (that is, in the “data” directory), but the path to the directory that contains the “data” directory.</p> <p>Adjust the “Log Level” slide bar to get more or less information presented in the “Event Log” window.</p>
Default appearance	<p>Here you can specify the default name, buffer size, fonts and colours that are used for new Console windows. You can also set the default directory where log files and workspace files are saved.</p> <p>To change the name, buffer size, fonts and colours for a specific Console window, right-click on the label for that particular Console and select “Properties” from the pop-up menu.</p>
Console Mode>Plotting	<p>Here you can change the default settings for any diagrams that will be plotted. When you make a new plot, it will be configured according to these settings. Existing plots are not affected by changes in these default settings.</p> <p>Note that these settings are shared with the Thermo-Calc Graphical mode. Any changes you make here will also apply to the default settings on the Graphical Mode>Activities>Plotting tab in the “Options” window (and vice versa).</p>

	<p>You can change the settings for individual plots that already exists in the Console Results window, by right-clicking the plot and selecting “Properties” from the pop-up menu.</p> <p>In addition, the colour, stroke (solid/dashed/dotted/dash_dot) and line width of a particular series of lines in a plot can be changed by double-clicking on one of the lines in that series.</p>
--	---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------

2.6 Database checker

The Thermo-Calc software package includes a program for checking that the syntax of Thermo-Calc database files is correct. This program is intended for users who develop and manage database. As a normal user of Thermo-Calc, you will probably never need to use the program.

To launch the DatabaseChecker application, select “Database Checker” from the “Tools” main menu.

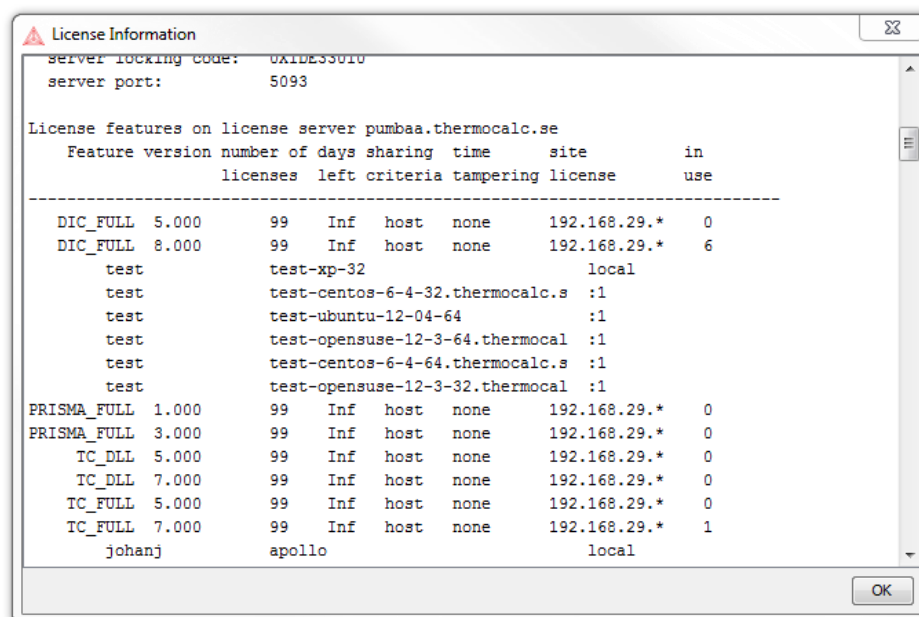
2.7 License information

To show information about the licenses you have for using Thermo-Calc, do either of the following:

- Use the SYS module command `DISPLAY_LICENSE_INFO`. Information about your license will be presented directly in the console.
- Select “Show License Info” from the “Help” main menu. This will open the License Information window.

If you are running a network client installation of Thermo-Calc, you can see how many of the client instance licenses that are currently “checked out” and how many of them that are left. You can also see which clients computers it is that have checked these client instance licenses out. If there are no such instances left, then you cannot enter the POLY module in Thermo-Calc.

The following screenshot shows an example of the kind of information that the License Information makes available on a network client installation. The table shows the various license types that the license server makes available (in this case, the license server is “pumbaa.thermocalc.se”).



The “number of licenses” column shows how many instances of each license type that can be checked out simultaneously, and the “in use” column shows how many of those instances that are currently checked out.

Under each license type with instances checked out, a list of who has checked out each of those instance is also shown. A license instance is checked out when you enter the POLY module and is checked back in when you leave the POLY module. In Graphical Mode, a license instance is checked out when an Equilibrium Calculator activity is created, and checked back in when the Equilibrium Calculator is removed.

For example, in the preceding screenshot, you can see that the user “johanj” has checked out a TC_FULL license.

2.8 Workflow

Working with Thermo-Calc involves moving between different modules. The workflow will differ depending on the kind of calculation you want to perform:

- 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. This workflow is described below. (However, 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 will prompt you to go through each step necessary for performing 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 plotting in various ways and save the diagram in various formats.

- If you want to tabulate a chemical substance, phase, or reaction, go directly to the TAB module. For more information, see section 4.9.

2.8.1 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, if you want to go to the DATA module, type the following:

```
GOTO_MODULE DATA
```

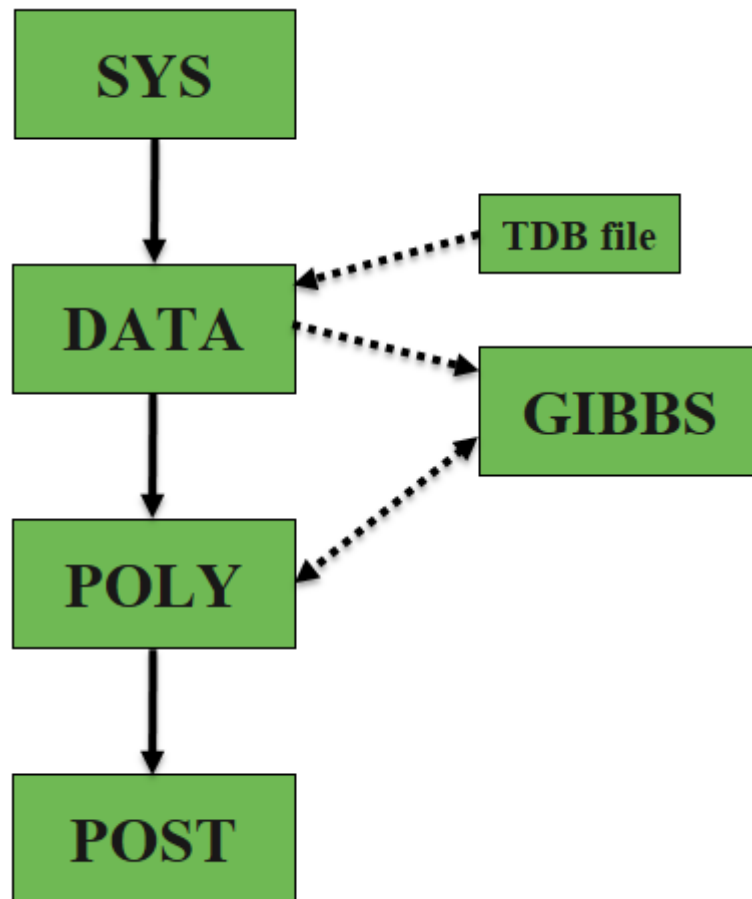
The exceptions are the submodules POST and ED-EXP. To go to the POST module, you must use `POST`, a command that is only available in the POLY module. To go to the ED-EXP module, you must use `ED-EXP`, a command that is only available in the PARROT module.

To go back to the module you came from when entering the module you are currently in, use `BACK`. For example, if you entered the DATA module from the SYS module and use `BACK`, you will go back to the SYS module. Note that you must use `BACK` to leave the submodules POST and ED-EXP. The `GOTO_MODULE` command is not available in these submodules.

Note that if you do not have a valid Thermo-Calc license, then you cannot leave the SYS module. To enter the DICTRA and DIC_PARROT modules, you also need a valid DICTRA license key.

2.8.2 Typical workflow when using POLY

The following figure 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 movement of data within Thermo-Calc.



The basic workflow is the following:

- 1 When you start Thermo-Calc in the Console Mode, you find yourself in the SYS module.
- 2 Define your system in the DATA module: Before performing your calculation, you must define your system and retrieve thermodynamic data. See chapter 0 for more information. The data is retrieved from a database file (*.TDB or *.TDC), and the data needed for describing your system is sent to the GIBBS module. This data is then accessed by the POLY module when you instruct it to perform calculations.
- 3 Perform the calculation in the POLY module: In POLY, you first set the conditions for an equilibrium calculation (temperature, pressure, system composition, etc.), then do the equilibrium calculation. If you want to go on and make a property or phase diagram, you set the conditions for a stepping or mapping operation and perform that operation. This will generate data that can be used to plot a property diagram (if you performed a stepping operation) or a phase diagram (if you performed a mapping operation). See chapter 4 for more information.

- 4 Plot and visualize your data in the POST module: If you have performed a stepping or mapping operation, then you can go to the POST module and plot a property of 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 in a host of ways. You can save the diagram either as a plain text file with data about all the coordinates or as an image file (in many different formats). See chapter 0 for more information.

3 Defining a system

Selecting the chemical components on which a calculation is to be run is called defining a system. To do this, you need to make use of some database(s) with thermodynamic, and then define which elements that your system will have as components. Once you have defined your system, you have to retrieve thermodynamic data for the system from the database(s).

If you use a response-driven module to perform your calculation, such as BIN or POURBAIX for example, then that module will prompt you to select database(s) and define your system. When performing calculations in the POLY module, you will typically have to manually select databases and define your system in the DATA module. This section describes how to do this. However, note that it is also possible to define the system directly in POLY using `DEFINE_MATERIAL` and `DEFINE_DIAGRAM` (see the *Thermo-Calc Console Mode Command Reference* for information about these commands).

3.1.1 How to define your system

To define your system means to select its components and to retrieve thermodynamic data about those components from an appropriate database. This section describes how you do this in the DATA module.

Pre-requisites

To define your system, you must be in the DATA module. Use `GOTO_MODULE DATA` to enter it.

Procedure

To define your system, follow these steps:

Step	Action
1	<p>Use <code>SWITCH_DATABASE</code> to change your default database. Unless you directly specify the name of the database as a parameter to the command, then the available databases will be listed, and you will be prompted to specify which you want to use.</p> <p>The second part of the command prompt indicates the current default database. For example, if the prompt reads “TDB_TCFE7:”, then this means that the current database is TCFE7.</p>
2	<p>Use <code>DEFINE_ELEMENTS</code> 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 <code>LIST_DATABASE ELEMENTS</code>.) For example, if you want to have Fe and C in your system, you would type:</p> <pre>DEFINE_ELEMENTS Fe C</pre>
3	<p>Use <code>REJECT PHASES</code> if you want to avoid retrieving any phases from the database. (To list the phases that are available in your current database, use <code>LIST_DATABASE PHASES</code>. To list the phases that can form in the defined system, use <code>LIST_SYSTEM CONSTITUENT</code>.) For example, if you do not want the graphite phase to be retrieved, you would write:</p> <pre>REJECT PHASES GRAPHITE</pre>

If the number of phases that should be included is much lower than the total number of phases, then it may be convenient to first reject all phases using `REJECT PHASES *` and then restore the phases that should be included using `RESTORE PHASES`.

- 4 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.

- 5 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.
- 6 Define your elements and specify whether to reject and restore any phases. Do this in exactly the same way as you would using the `SWITCH_DATABASE` command (see the preceding steps 2 and 3).
- 7 Use `GET_DATA` to search the database and add the thermodynamic data to the data that already exists in the GIBBS workspace.

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.

4 Calculation

This chapter describes some of the most common calculations performed in Thermo-Calc. Calculations can be performed either in the POLY module, or using some of the response-driven modules that have been designed to enable you to perform some specific type of calculation.

The first three sections of this chapter describes, in very general terms, how to perform an equilibrium calculation, calculate and plot a property diagram, and calculate and plot a phase diagram. There is an endless variety of calculation types that can be plotted as property or phase diagrams. What follows are descriptions of a basic kind of calculation. At each section, a few ways in which you can change settings or conditions are also described.

Note that to calculate and plot a property diagram or a phase diagram, you must first calculate an equilibrium. The first section therefore describes how to calculate a single-point equilibrium.

4.1 Equilibrium

An equilibrium describes what the composition of the end state of your system will be, given a full specification of state variables such as temperature, pressure, initial composition, system size, etc. An equilibrium calculation is normally performed in POLY according to the Global Minimization Technique, which assures 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(LIQ,S)-X(PYRR,S)=0").

The number of state variables that needs to set is determined by the Gibbs Phase Rule (see *Educational Material*). Typically, the state variables that you need to give values to are the following:

- 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 state variables that are available and that you can use to set conditions:

State variable	SET_CONDITION parameter
temperature in the system (in K)	T

pressure in the system (in Pascal)	P
system size (mole number in moles)	N
system size (mass in grams)	B
number of moles of a component in the system	N(<component>)
mole fraction of a component in the system	X(<component>)
mass fraction of a component in the system	W(<component>)
activity of a component in the system	ACR(<component>)
chemical potential of a component in the system	MUR(<component>)
mole fraction of a component in a phase	X(<phase>,<component>)
mass fraction of a component in a phase	W(<phase>,<component>)
activity of a species referred to a phase at ambient temperature and pressure	ACR(<species>,<phase>)
chemical potential of a species referred to a phase at ambient temperature and pressure	MUR(<species>,<phase>)
enthalpy in the system (in J)	H
enthalpy of a phase (in J/mol)	HM(<phase>)

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 will detect this simply by failing to reach equilibrium during the calculation.

Here is an example of the kind of information about the equilibrium that will normally be presented to you:

```

POLY_3:1-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium =      1, label A0  , database: TCFE7

Conditions:
T=1000, P=1E5, X(C)=5E-2, N=1
DEGREES OF FREEDOM 0

Temperature  1000.00 K (  726.85 C),  Pressure  1.000000E+05
Number of moles of components  1.00000E+00,  Mass in grams  5.36552E+01
Total Gibbs energy -4.07975E+04,  Enthalpy  2.41176E+04,  Volume  7.21740E-06

Component              Moles      W-Fraction  Activity   Potential  Ref.stat
C                      5.0000E-02  1.1193E-02  2.1816E-01 -1.2659E+04 SER
FE                     9.5000E-01  9.8881E-01  6.1895E-03 -4.2279E+04 SER

BCC_A2                  Status ENTERED      Driving force  0.0000E+00
Moles 9.5069E-01, Mass 5.3063E+01, Volume fraction 9.6312E-01  Mass fractions:
FE 9.99844E-01  C  1.55514E-04

GRAPHITE                  Status ENTERED      Driving force  0.0000E+00
Moles 4.9313E-02, Mass 5.9230E-01, Volume fraction 3.6881E-02  Mass fractions:
C  1.00000E+00  FE  0.00000E+00

```

4.1.1 How to calculate 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.

Pre-requisites

Before calculating an equilibrium, you must have defined your system and entered POLY. Note that 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. See sections 2.6 and 1.4 for more information.

Procedure

To calculate an equilibrium, follow these steps:

Step	Action
------	--------

- 1 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.

- 2 Use COMPUTE_EQUILIBRUM to run the calculation.

- 3 Use LIST_EQUILIBRIUM to see the results of the calculation.

4.1.2 Variations

There are many possible variations on how an equilibrium can be calculated in Thermo-Calc. Here is one possible variation that you may find useful.

Calculating an equilibrium with a fixed phase

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 your system will start to melt, then 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 will include the value of the unspecified variable at which the equilibrium enters the phase that you hold fixed.

For an example where an equilibrium is calculated with a fixed phase, see Example 7 in the *Thermo-Calc Console Examples Collection*.

Calculating an equilibrium with suspended or dormant phases

You can calculate an equilibrium under the assumption that one or several phases are suspended ("SUSPENDED") or dormant ("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 the *Thermo-Calc Console Examples Collection*.

4.2 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 will be referred to as the stepping axis variable. In Thermo-Calc, you 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 you have specified.

For an example of the calculation of a property diagram, see Example 8 in *Thermo-Calc Console Examples Collection*.

4.2.1 How to calculate and plot 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 will retain their values when the new equilibria are calculated.

Pre-requisites

To calculate a property diagram, you should first have calculated an initial equilibrium. You must also be in the POLY module. For information about how to calculate an equilibrium, see section 4.1.

Procedure

To calculate a property diagram, follow these steps.

Step	Action
------	--------

- | | |
|---|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1 | 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 should be 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, you would enter |
|---|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

```
SET_AXIS_VARIABLE 1 T 100 2000 50
```

Note that an axis variable must be a state variable that you 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.

- | | |
|---|----------------------------------------------------|
| 2 | Use STEP NORMAL to perform the stepping operation. |
|---|----------------------------------------------------|

Thermo-Calc will list 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 which phases it contains. Note that the number of equilibria calculated will not simply be the number of steps that would be 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
```

- 3 To plot the diagram, use POST to open the POST module and then use PLOT. By default, the X-axis will represent the stepping axis variable and Y-axis will represent the sum of the mole fractions of all phases (NP(*)). See chapter 0 for more information about visualization.

4.2.2 Variations

There are many possible variations on how a property diagram can be calculated in Thermo-Calc. Here are some possible variations that you may find useful.

Calculating a property diagram one phase at a time

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.

Calculating several properties in the same diagram

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 could 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 could 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 could be useful.

Unless you have opened a new workspace file previously using SAVE_WORKSPACES, the results of the stepping calculations will be saved in a RESULT.POLY3 file. If you want 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. Note that SAVE_WORKSPACES overwrites and deletes the results of all previous stepping calculations!

4.3 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 will be 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 subsections describe how you calculate different 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 may combine activity conditions and fixed phase status and fraction conditions in any way. Thermo-Calc can calculate any arbitrary two-dimensional section through composition space. Note that there is no guarantee that the conditions you have 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 the *Thermo-Calc Console Examples Collection*.

4.3.1 How to calculate and plot a phase diagram

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

Pre-requisites

Before calculating a phase diagram, you must first have calculated an initial equilibrium. You must also be in the POLY module. For information about how to calculate an equilibrium, see section 4.1.

Procedure

To calculate a phase diagram, follow these steps:

Step	Action
------	--------

- 1 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 should be 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 would then enter:

```
SET_AXIS_VARIABLE 1 W(C) 0 .1 0.002
```

Note that an axis variable must be a state variable that you 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.

- 2 Use SET_AXIS_VARIABLE to set the second axis variable and specify its minimum, maximum, and step length values. The axis number should be 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 would then enter:

```
SET_AXIS_VARIABLE 2 T 900 1900 25
```

- 3 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 will save the axis variables you have set. However, note that it will overwrite the results of any previous stepping or mapping calculations you have done.

- 4 Use MAP to perform the mapping calculation.

The console will list 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
```

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

4.3.2 Variations

There are many possible variations on how a phase diagram can be calculated in Thermo-Calc. Here are some possible variations that you may find useful.

Calculating a quasi-binary phase diagram

A quasi-binary phase diagram is a phase diagram 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 will be 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 will have 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 would then enter:

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

For an example of a calculation of a quasi-binary phase diagram, see Example 17 in *Thermo-Calc Console Examples Collection*.

Calculating a quasi-ternary phase diagram

A quasi-ternary phase diagram is a 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 could 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
```

4.4 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.

In Thermo-Calc, you can simulate Scheil-Gulliver solidification processes with the SCHEIL module. When you enter the module, you will be prompted to answer a series of questions about which database to use, what the major element is and in which amount. Thermo-Calc will then present you with a property diagram that shows how the fraction of solid phase varies with temperature (in Celsius). You can then plot diagrams using other variables that 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, or by opening an old file that you base a new simulation on using a different bulk composition. 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.

The following subsection describes how to perform a simulation of a Scheil-Gulliver solidification using the SCHEIL module both with and without back-diffusion.

There are several examples in the *Thermo-Calc Console Examples Collection* that you may consult for more information on how the SCHEIL module can be used:

- For examples of using the SCHEIL module to simulate non-equilibrium transformations without considering fast-diffusion elements, see Examples 15 and 30.
- For an example of using the SCHEIL module to simulate partial-equilibrium transformation with fast-diffusion elements taken into consideration, see Example 48. This example also shows how you can perform lever-rule calculations (full-equilibrium transformations).

4.4.1 How to simulate 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).

Pre-requisites

None.

Procedure

To simulate a Scheil-Gulliver solidification, follow these steps:

Step	Action
1	Use GOTO_MODULE SCHEIL to enter the SCHEIL module.
2	Type "1" to "Start new simulation".
3	Specify which database you want 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 superalloy, enter Ni.
5	Set whether to specify the composition of your system in mass (weight) percent or in mole percent. Enter "Y" for mass percent and "N" for mole percent.
6	Specify the name of the first alloying element. You can directly specify mass or mole percent after the name (for example, you may enter "Cr 5"). If this is not specified, then you will be prompted to enter it separately.

- 7 Specify the other alloying elements in the same way as you specify the first. After you have specified your last alloying element, simply press the enter-key when requested to specify the next element. This will end the process of defining the bulk composition of the alloy system.

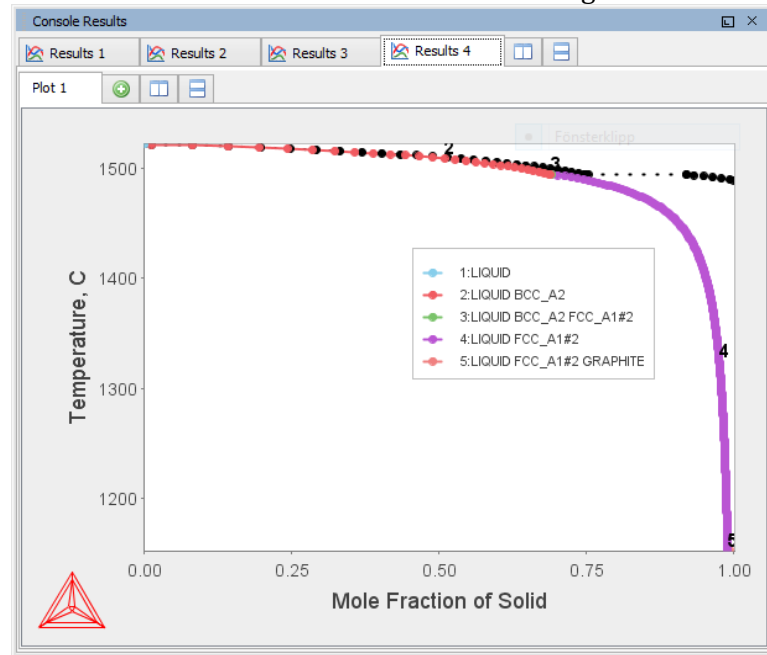
You can also specify all the alloying elements and their corresponding compositions on the same line when you are prompted to specify your first alloying element in Step 6 above. For example, you could enter "Cr 5 Ni 1 Mo 0.5 C 0.01 N 0.02".
- 8 Specify the starting temperature in Celsius.

This value should be sufficiently high so that the solidification simulation starts with the alloy system in the liquid single-phase region.
- 9 Decide which phases (if any) that you want to reject. You will be prompted to enter the name of the phases you want to reject until you press the enter-key.
- 10 Decide which phases (if any) to restore. 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.
- 11 When prompted with "OK?" type "N" if you want 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 have defined is now retrieved from the database.
- 12 Specify whether any phases should have a miscibility gap check. If you answer Y, you will be prompted to specify the solution phase name(s) as well as the major constituents on each of their sublattice sites. When you are done, press the enter-key when prompted to specify another phase.

The module now calculates and presents the real liquidus temperature for the defined alloy system.
- 13 Specify the temperature step. This sets how much the temperature will decrease at each step in the simulation.
- 14 Decide whether you want to use a default stop point or define your own. By default, the simulation stops when the mole fraction of the remaining liquid phase is approximately 0.01. If you choose to not use this point, then you will be prompted to specify whether you want to define the stop point in terms of approximate fraction of liquid phase or in terms of approximate temperature (in Celsius).
- 15 Specify the names of any fast-diffusing components. Type all the names on the same line before pressing the enter-key. If you do specify any fast-diffusing components, then you will be prompted to set whether BCC to FCC phase transformations should be simulated.
- 16 You will now be asked to specify the name of the POLY3-file that the simulation results will be saved to.

The Scheil-Gulliver solidification simulation will now run, and the default diagram (Temperature versus Mole Fraction of Solid) will automatically be plotted in the Console Results window. The screen shot below shows one such default diagram.



- 17 Answer questions concerning how the graph is plotted and how the results of your simulation should be saved. You will be asked whether to do any of the following:
- print the diagram (save a hard copy)
 - save the X- and Y-coordinates of the plotted diagram in an EXP-file
 - plot more diagrams from the same simulation results.

4.4.2 How to plot additional Scheil simulation diagrams

If you have done a Scheil-Gulliver solidification simulation and plotted the default diagram (Temperature versus Mole Fraction of Solid), then you can plot additional diagrams based on the results of that simulation but with different variables as axes.

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.

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

Pre-requisites

You must have already run a Scheil simulation to plot a diagram with other variables than Temperature and Mole Fraction of Solid on the Y-axis and the X-axis. You can either plot such additional diagrams directly after having finished the simulation (at Step 19 in the procedure described in section 4.4.1), or by choosing option 2 ("Open old file and plot diagram") when you enter the SCHEIL module and opening a POLY3 workspace file.

Procedure

To plot the diagram, follow these steps:

Step	Action
1	Type "Y" when prompted about whether to plot another diagram, or select option 2 when you enter the SCHEIL module.
2	Specify which variable you want the X-axis to represent. Use the abbreviation specified in the preceding table. You can use the asterisk ("*") as a wild card character to select all elements (el) or phases (ph).
3	Specify which variable you want the Y-axis to represent. The diagram will be immediately plotted in the Console Results window.
4	Type "Y" or "N" to decide whether to zoom in on a specific area of the plotted diagram. If you type "Y", then you will be prompted to specify the scaling of the axes and their minimum and maximum values. The diagram is plotted again according to the values you have specified. You will then again be asked whether you want to zoom in again. Continue to zoom in until you are satisfied with the presented plot.
5	Type "Y" or "N" to set whether to print the diagram (save a hard copy).
6	Type "Y" or "N" to set whether to save the X- and Y-coordinates of the plotted diagram in an EXP-experimental data file (this is a plain text-file).
7	Type "Y" or "N" to decide whether to plot more diagrams using the results of the same simulation. If you enter »Y«, then you will start over from Step 2.

4.4.3 How to run additional simulations on your alloy system

If you have already run a Scheil simulation, you can run additional simulations on the same alloy system. This allows you to change the system composition, the temperature, the amount of temperature decrease at each step, and the approximate stop point of the simulation.

If you want to change the database used, the components of your alloy system, change whether the fraction of the components are specified in mass or mole, or reject or restore different phases, then you must run a completely new simulation from scratch (see section 4.4.1 for information how to do that).

Pre-requisites

You can only run an additional Scheil simulation if you have a POLY3 workspace file in which a previous Scheil simulation has been saved.

Procedure

To run an a new simulation base on the a previous simulation, follow these steps

Step	Action
1	Use GOTO_MODULE SCHEIL to enter the SCHEIL module.
2	Type "3" to "Open old file and make another simulation".
3	Specify the fraction of the first alloying element. Whether you are prompted to specify it mass or mole fraction depends how you specified it in the first simulation. If there are more than one alloying elements, you will be prompted to specify the fraction of each of them before you proceed to the next step.
4	Specify the starting temperature in Celsius.
5	Enter the length of the temperature step. This sets how much the temperature will decrease at each step in the simulation.
6	Decide whether you want to use a default stop point or define your own.
7	Specify the names of any fast-diffusing components. The Scheil-Gulliver solidification simulation will now run, and the default diagram (Temperature versus Mole Fraction of Solid) will automatically be plotted in the Console Results window.
8	Type "Y" or "N" to set whether to print the diagram (save a hard copy).
9	Type "Y" or "N" to set whether to save the X- and Y-coordinates of the plotted diagram in an EXP-experimental data file (this is a plain text-file).
10	Specify whether you want to plot more diagrams using the results of your simulation. For information about how to plot additional diagrams, see section 7. If you enter »N«, then you will exit the SCHEIL module.

4.5 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 will often be 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.

4.5.1 How to make a T0 temperature simulation

This section describes how to perform a T0 temperature simulation and apply a stepping calculation to its initial result.

Pre-requisites

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.

Procedure

To perform an initial T0 temperature simulation and then a stepping calculation based on this initial simulation, follow these steps:

Step	Action
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) will be presented 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 that should be used as the stepping variable. This is done in exactly the same way as when you calculate a normal property diagram, see section 4.2.1. Note that when you run a T0 temperature simulation, you cannot set temperature as the stepping variable.

- 7 Use STEP T-ZERO to initiate the stepping calculation. You will be prompted to specify the names of the target phases for which the T0 temperature will be 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 the *Thermo-Calc Console Examples Collection*. For more information about visualization, see chapter 0.

4.6 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 will be equal in such a case, but this will not be 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.

4.6.1 How to calculate a paraequilibrium

This section describes both how to calculate an initial paraequilibrium with two target phases, and how to base a stepping calculation on this initial calculation.

Pre-requisites

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.

Procedure

To calculate an initial paraequilibrium and do a stepping calculation based on it, follow these steps:

Step	Action
------	--------

1	Use SET_CONDITION to set the conditions of your calculation just like when you calculate an ordinary equilibrium.
---	-------------------------------------------------------------------------------------------------------------------

2	Use CHANGE_STATUS_COMPONENT to set the status of the chosen interstitial components to SPECIAL. For example, if C is an interstitial component, enter:
---	--------------------------------------------------------------------------------------------------------------------------------------------------------

```
CHANGE_STATUS_COMPONENT COMPONENTS C=SPECIAL
```

This will give 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 will not be 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_EQUILIBIRUM to run the calculation.
---	-------------------------------------------------

4	When you have calculated your initial equilibrium, use ADVANCED_OPTIONS 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".
---	------------------------------------------------------------------------------------------------------------------

Note that 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.
---	--------------------------------------------------------------------------------------------------------------------------------------------------------------------

Note that 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 you will be presented with a message similar to the following:

```
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 that should be used as the stepping variable. This is done exactly in the same way as when you calculate a normal property diagram. See section 4.2.1 for information about how to calculate a property diagram.
- 8 Use STEP PARAEQUILIBRIUM to initiate the stepping calculation. You will be prompted to specify the names of the target phases of the paraequilibrium states, and the names of the fast-diffusing components.

The stepping calculation is performed, and the different phase regions will be 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 screen shot shows an example of the kind of information that will be listed:

```
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 general information about visualization, see section 0. For an example of a paraequilibrium calculation and how it can be plotted, see Example 23 in the *Thermo-Calc Console Examples Collection*.

4.7 Potential diagrams

If you have a metal-oxide/sulfide-gas interaction system, you might want to calculate a so-called potential phase diagram given certain temperature and pressure. A potential diagram use 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-sulfides, 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 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.

4.7.1 How to calculate a potential diagram in POTENTIAL

Pre-requisites

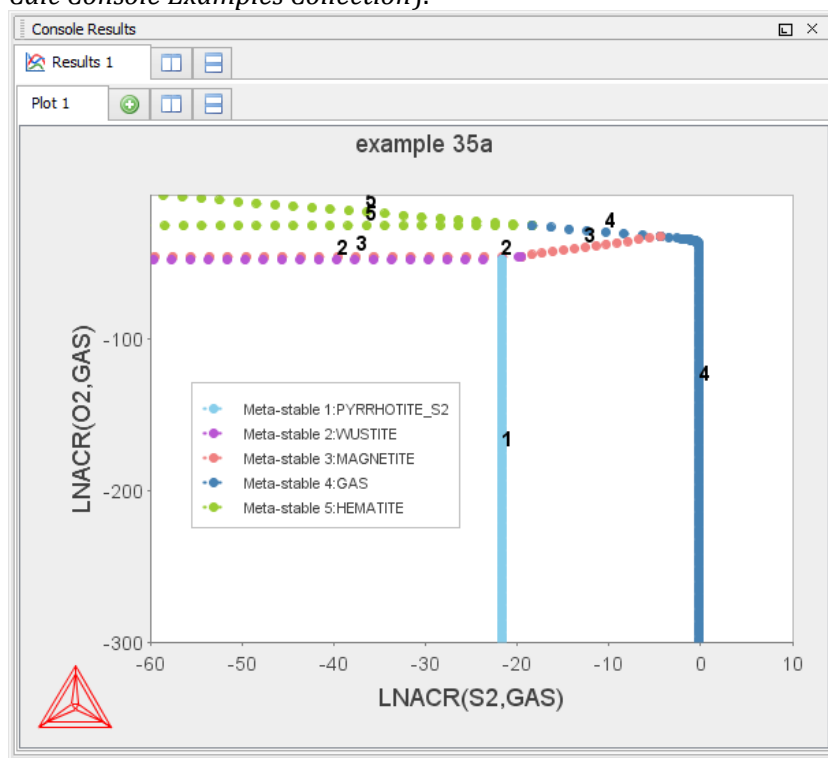
You need access to a substance or solution database that contains a gaseous mixture phase, metals (or alloys), and solids such as metal-oxides, sulfides, sulfates, carbonates, silicates, nitrides or nitrates (stoichiometric or solution phases). You can always use the TC Public Substances Database (PSUB),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

Procedure

To calculate a potential diagram, follow these steps:

Step	Action
1	Use GOTO_MODULE POTENTIAL to enter the POTENTIAL module.
2	Specify which substance or solution database that should be used. Any substance or solution database can be used that has a gaseous mixture phase, metals (or alloys), and solids such as metaloxides, sulfides, sulfates, carbonates, silicates, nitrides, and nitrates (stoichiometric or solution phases).
3	Specify the matrix element (a metal) and the two gaseous species that define you metal-gas interaction system. The names of these components must be available in the database you are using.
4	Set the temperature (in Kelvin). (The pressure is always 1 bar.)

A potential diagram with the activities of the two gaseous species as mapping variables is calculated. These mapping variables are also set as the axis variables in the plotted diagram. The following screenshot is one such diagram (from example 35 in the *Thermo-Calc Console Examples Collection*).



A POLY3-file is also automatically saved in the current working directory with the default name POT.POLY3.

- 5 When the diagram has been plotted, it opens the POST module where you can modify the plotted diagram in any way you like. For information about the POST module, see chapter 0.

4.7.2 How to calculate 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. This will be useful if you want to calculate a potential diagram at a pressure other than 1 bar for example.

This section describes how you calculate a potential diagram in which the pressure is set to a different value than 1 bar.

Pre-requisites

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

Procedure

To modify a potential diagram in POLY, follow these steps:

Step	Action
------	--------

- 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 will open that workspace file and load the previous settings and results. The activities of the two gaseous species will now be part of your conditions, and these conditions will be set as your mapping variables.
- 3 Use SET_CONDITION to specify the pressure under which you want the potential diagram to be calculated. For example, if you want the pressure to be 1000 bar, then 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 will be 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. See section 0 for information about visualization.

4.8 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, sulfides, sulphates, nitrates, silicates, carbonates and other solids, or gaseous mixtures, will be 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 H₂O, 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 ₂ O	ENTERED	AQUEOUS	*	100000
H+1	ENTERED	SER		
ZE	ENTERED	REFERENCE_ELECTRODE	*	100000

Besides the aqueous solution phase, your system may also contain a gaseous mixture phase. Other neutral and charged gaseous species may also be constituents. For multicomponent systems there should normally also be 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 should contain at least the AQUEOUS and REFERENCE_ELECTRODE phases. The aqueous solution database need to be appended with additional required data and phases, such as various interacting alloy (solid) solution phases and various secondary (solid and liquid) phases. Additional data will come from one or more databases, such as SSUB/SSOL/TCFE or other substances/solutions databases.

4.8.1 How to calculate 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.

Pre-requisites

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.

Procedure

To calculate a Pourbaix diagram, follow these steps:

Step	Action
1	Use GOTO_MODULE POURBAIX to enter the POURBAIX module.
2	Type "1" to "Start a completely new POURBAIX diagram calculation", or type "3" to "Open an old file & make another POURBAIX stepping calculation"
	To choose this third option, you must have already done a Pourbaix calculation and have it saved in a POLY3-file. The new calculation will use the same system definition as the previous calculation, but you can modify the other conditions such as the bulk composition, temperature and pressure in the next step.
3	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 ₂ O, 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.
4	Type "Y" or "N" to set whether to use a single database or a multiple database.
	If you choose to use a single database, you then need to specify a database that has been specially developed for the POURBAIX module's diagram calculations. If you choose to use a multiple database, then you will be prompted to specify an aqueous solution database and then to append any additional required data and select necessary phases, such as various interacting alloy (solid) solution phases, and various secondary (solid and liquid) phases for example.

- 5 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). Note that 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, simply press the enter-key when asked to specify "Next solute".

The definition of your system and its initial bulk composition is now presented.

- 6 Type "Y" to confirm the defined system and its bulk composition.

The thermodynamic data for your system will now be retrieved from the database(s) you have chosen.

- 7 Answer the questions that you are prompted with regarding various parameters of your calculation. You will be asked whether to do any of the following:

- reject or restore any phases
- check for miscibility gaps on any phase
- enforce the Global Minimization Technique in all calculations
- save your functions, variables and tables in a POLY3-file
- set any numerical limits on the calculation
- accept the default settings for the two mapping variables

The Pourbaix calculation will now be performed and the Eh-pH diagram plotted.

- 8 Type "Y" or "N" to set whether you want to add starting points to the calculation. If you suspect that the calculation has missed some phase boundaries, this may help the program to detect them.

- 9 Answer questions concerning how the diagram is plotted and how the results of your calculation should be saved. You will be asked whether 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
- 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 Pourbaix diagram

4.8.2 How to plot 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 will be searched.

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)

Pre-requisites

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 (at the end of Step 4 in the procedure described in section 4.8.1), or by choosing option 2 ("Open an old file & plot other property diagrams") when you enter the POURBAIX module and opening a POLY3 workspace file.

Procedure

To plot the diagram, follow these steps:

Step	Action
------	--------

- | | |
|---|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 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 concerning how the diagram is plotted and how it should be saved. You will be asked whether 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

4.8.3 How to do a stepping calculation on 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.

Note that 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
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 will automatically calculate the equilibrium constant in logarithmic ($\log_{10}K_a$) of the electrolysis reaction H_2O (water) = $H^+ + OH^-$ 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, an increment factor with a default value should be confirmed or modified; for pressure and mole of a component, one can specify the step in logarithmic ($\log_{10}P$ or $\log_{10}N$).

Pre-requisites

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

Procedure

To make a stepping calculation on an aqueous solution, follow these steps:

Step	Action
1	Use GOTO_MODULE POURBAIX to enter the POURBAIX module.
2	Type "4" to "Open an old file & 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.

4.9 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.

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 (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.

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

4.9.1 How to tabulate 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.

Pre-requisites

None.

Procedure

To tabulate chemical substances, phases or reactions, follow these steps:

Step	Action
------	--------

- 1 Use GOTO_MODULE TAB to enter the TAB module.
- 2 If you want to add one thermodynamic function to the tabulation calculation, which will be present in a sixth column in the table, use ENTER_FUNCTION.

You will then be prompted to enter the name of the column that will be presented 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. The chemical reaction should be terminated with a semi-colon. For example, you could 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" will hence be interpreted as Cobalt rather than as carbon monoxide. Carbon monoxide should be 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 will be presented with a table that shows the various properties at each temperature level within the range you have 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 has been plotted, you end up in the POST module, where you can modify the graph in various ways. For more information about the POST module, see chapter 0.

4.9.2 How to tabulate 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.

Pre-requisites

None.

Procedure

To tabulate a substance or solution phase, follow these steps:

Step	Action
------	--------

- 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.

Note that 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 will be present in a sixth column in the table, use ENTER_FUNCTION.

You will then be 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 you will be presented with a table that shows the various properties at each temperature level within the range you have defined.

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 has been plotted, you end up in the POST module, where you can modify the graph in various ways. For more information about the POST module, see chapter 0.

5 Visualization

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 will be 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).

5.1 How to plot your diagram

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 the X- and Y-axes will by default represent the mapping axis variables 1 and 2 (which were 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 will represent the stepping variable (which was set using SET_AXIS_VARIABLE in POLY) and the Y-axis will be represent the sum of the mole fractions of all phases (that is, NP(*)).

Pre-requisites

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. Note that you use POST to enter the POST module (using GOTO_MODULE POST will lead to a “NO SUCH MODULE” message). The POST command is only available inside POLY.

Procedure

To plot a diagram, follow these steps:

Step	Action
------	--------

- 1 If you want to directly plot your diagram with the default variables represented by the X- and Y-axes, simply type PLOT and press the enter-key. This will plot a property or phase diagram with the default variables represented at each axis. If you do not want to plot your diagram using these default variables, go on to the next step.
- 2 Use SET_DIAGRAM_AXIS to set which variables that should be plotted 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, you would type:


```
SET_DIAGRAM_AXIS X T
SET_DIAGRAM_AXIS Y P
```
- 3 Use PLOT to plot your diagram.

5.2 Modifying your diagram

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 would simply use SET_DIAGRAM_AXIS to set diagram axis "Y" to "w(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 you make in the plot settings will be taken into account the next time you use PLOT.

The following are some of the modifications you can make. For more information on what you can do, see the *Thermo-Calc Command Reference*:

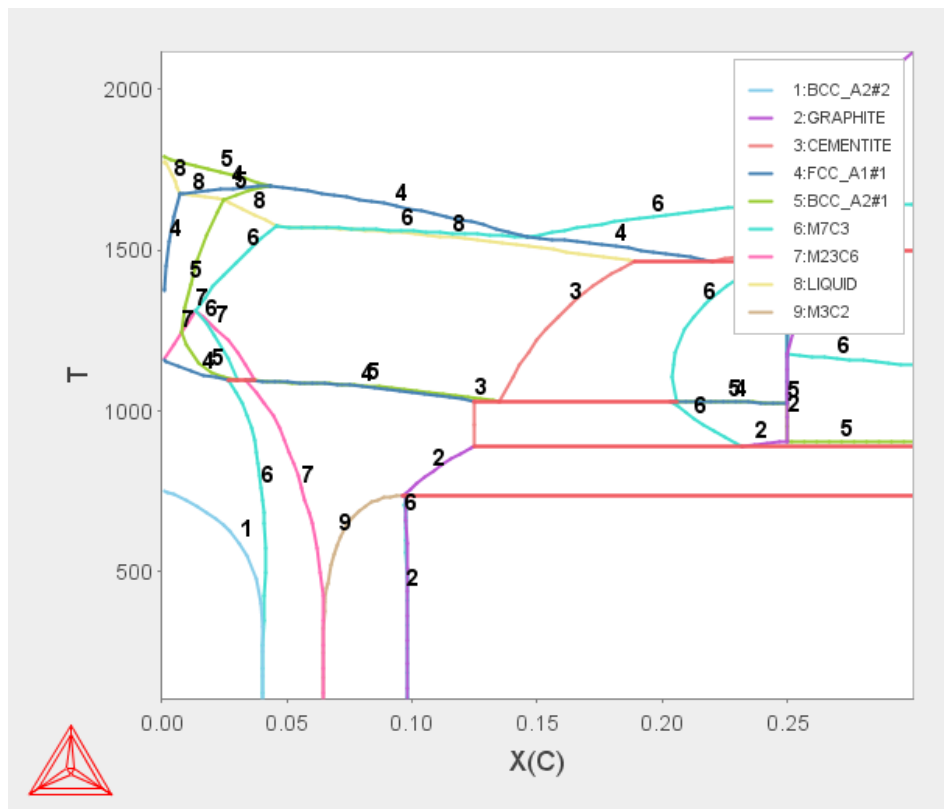
SET_TITLE	Use this to set add a title or to change an already existing title. The title will be displayed above the plotted diagram in the Console Results window.
ADD_LABEL_TEXT	Use this to add a label text that starts at a certain X- and Y-coordinate. If you have plotted a phase diagram, then you can let Thermo-Calc set the label text that specifies the names of the stable phases at that coordinate.
SET_AXIS_TYPE	Use this to set whether the scale of an axis should be linear, logarithmic or inverse.
SET_DIAGRAM_TYPE	Use this 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.
SET_SCALING_STATUS	Use this to modify the range of values that will be 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, you would type:

```
SET_SCALING_STATUS X N 0 0.3
```

The “X” specifies which axis to change the scaling on, the “N” turns on 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”.

```
SET_LABEL_CURVE_OPTION E
```

Use this to label each set of curves that have the same stable phases with a certain digit. A legend is also added, where it will be specified which phases each digit designates. The following screenshot shows how this might look:



5.3 Changing the appearance of your diagram

To change the appearance of your diagram, right click on the diagram and select “Properties” from the pop-up menu. This will open up a Plot Properties window. Here you can, for example, change the fonts and colours used, and enter a title for your diagram.

You can also change the colour, stroke (solid/dashed/dotted/dash_dot) and line width of a particular series of lines in the plot by double-clicking one of the lines in the series. In this way, you can also toggle whether data points should be shown or not for a series of lines. The crosshair cursor turns into a cursor resembling a pointing hand when it is placed over a line that can be clicked but if you hold down Ctrl, this will not happen (the cursor will continue to be shown as a crosshair).

To configure the default settings for plotting, select “Options” from the “Tools” main menu and open the “Plotting” tab under Console Mode.

5.4 Saving your diagram

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

`MAKE_EXPERIMENTAL_DATAFILE`

Use this 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. See the *DATAPLOT User Guide* for more information. Note that information about the underlying calculations that the diagram is based on is not saved in an EXP-file.

`DUMP_DIAGRAM`

Use this to save the diagram image to a PS, PDF, SVG, EMF, GIF, or PNG file. You will be asked which format to save it.

Right click on diagram | Save Plot

Do this to save the diagram image in a variety of image file formats.

`PRINT_DIAGRAM`

Use this to print a hard copy of the diagram.

5.5 Loading a previously saved diagram

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 should be loaded from an experimental data file. For more information about EXP-files and the DATAPLOT graphical language, see the *DATAPLOT User Guide*.

`APPEND_EXPERIMENTAL_DATA`

Use this 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 will not be changed when you plot the additional data from the EXP-file, irrespectively of the data in that file.

`QUICK_EXPERIMENTAL_PLOT`

Use this to plot selected data from an experimental data file (EXP-file). If you have set the axes of the diagram already, these settings will be overwritten with the axes settings from the EXP-file.

6 Appendix 1 – Thermodynamic variables and units

The following appendix contains information about different thermodynamic variables recognised by Thermo-Calc. Section 6.2 contains information on how to define new derived variables and functions. Finally, section 7.3 presents information that is useful if you want to express thermodynamic variables in non-default units. The POLY module only recognises default units, which are the SI units.

6.1 Thermodynamic variables

There are different kinds of thermodynamic variables in Thermo-Calc. Some are state variables such as temperature, pressure and mole fraction. These characterize the equilibrium state of a system. You set them when you define your system in the POLY module before performing a calculation. They are also used in other modules such as DATA, GIBBS and PARROT. State variables that involve components can be used for the defined components, but not for any species. (To define new components in a defined system, use `DEFINE_COMPONENT`).

Other useful thermodynamic variables are derived from state variables with a mathematical function. Some derived variables are pre-defined by Thermo-Calc, such as normalized energetic and compositional extensive state variables for example. You use these by appending various normalizing suffixes to abbreviations that are associated with the state variables.

Thermodynamic variables can also be divided into extensive variables and intensive variables. An extensive variable is a variable whose value depends on the size of the system, whereas an intensive variable is a variable whose value is independent of system size.

More information about thermodynamic variables is available in the online help in Thermo-Calc Console Mode. Use the `INFORMATION` command, with a subject keyword such as one of the following as argument: `STATE VARIABLES`, `INTENSIVE VARIABLES`, `EXTENSIVE VARIABLES`, `DERIVED VARIABLES`, `CONDITIONS` (for condition settings), `AXIS-VARIABLES` (for stepping/mapping variable settings).

6.1.1 Table of thermodynamic variables

The table below lists common thermodynamic variables. Most of these can be used to define equilibrium conditions in the POLY module. If this is not the case, then this is stated in the “Comment” column.

The “Abbrev.” column shows the abbreviation that you use in the POLY module for referring to the variable. If the variable must be given any arguments, then these are given in parenthesis directly after the abbreviation. For most variables, this is also the abbreviation that you use to refer to the variable in other modules. However, some variables are referred to with a different abbreviation in the POST module. If this is the case, then this is noted in the “Comment” column.

Variables that are specific to a species, in which case the species should be specified as an argument (“sp” in the table below). Note that if there are two or more sublattices in a given phase, then this argument should be given as “constituent#sublattice”. This indicates a constituent on a specific sublattice or site in the phase (referred to by the ‘#’ sign and a digit). For instance, “y(BCC,C#2)” stands for the site fraction of the C species on the second sublattice site of the BCC_A2 solution phase.

The “Unit” column show which unit that you can use to express the variable in the POLY module. This unit is always the SI unit. In other modules, state variables may be expressed in other units. For more information, see section 6.3.

The “Suffix” column shows which suffixes that you can append to the variables. The “R”-suffix can be used with all compositional extensive state variables, but the suffix will not change the value of the variable. This has been indicated by putting the “R” in parenthesis.

V	Abbrev.	Unit	Descript.	Domain	Comment	Suffix
Intensive variables						
T	T	K	Temperature	System	When plotting in POST, besides “T” (Kelvin), you can also use “T_C” or “T_F” to plot temperature in °C or °F.	
P	P	Pa	Pressure	System		
μ	MU(comp)	J/mol	Chemical potential	Component		R
	MU(sp,ph)			Species relative to a solution phase	Only for single-substitutional-lattice solution phases such as AQUEOUS solution and GASEOUS mixture phases and for interacting species on the the substitutional sublattice of two-sublattice solution phases (such as the phases BCC_A2 and M6C phases).	R
a	AC(comp)	N/A	Activity	Component		R
	AC(sp,ph)			Species relative to a solution phase	Only for single-substitutional-lattice solution phases such as AQUEOUS solution and GASEOUS mixture phases and for interacting species on the the substitutional sublattice of two-sublattice solution phases (such as the phases BCC_A2 and M6C phases).	R

V	Abbrev.	Unit	Descript.	Domain	Comment	Suffix
	LNAC (comp)		ln(Activity)	Component	In natural logarithm (lnAC=MU/RT)	R
	LNAC (sp,ph)			Species relative to a solution phase	In natural logarithm (lnAC=MU/RT) Only for single- substitutional-lattice solution phases such as AQUEOUS solution and GASeous mixture phases and for interacting species on the the substitutional sublattice of two- sublattice solution phases (such as the phases BCC_A2 and M6C phases).	R
Energy-related extensive variables for whole system or for a phase						
V	V	m3	Volume	System		M, W, V, R
	V(ph)			Phase	If phase is unstable, then V(ph) gets a value of zero.	M, W, F, R
	VP(ph)			Phase	VP(ph) should not to be used as a condition in POLY. Instead, use CHANGE_STATUS PHASE <PHASE>=FIX <AMOUNT> where the fixed <AMOUNT> is roughly equal to VPF(ph), which cannot be directly evaluated or listed. If the phase is unstable, then VP(ph) and its normalized quantities get zero value.	M, W, V, R
G	G	J	Gibbs energy	System		M, W, V, R
	G(ph)			Phase	If phase is unstable, then G(ph) gets a value of zero.	M, W, V, F, R
A	A	J	Helmholtz energy	System		M, W, V, R
	A(ph)			Phase	If phase is unstable, then A(ph) gets a value of zero.	M, W, V, F, R
U	U	J	Internal energy	System		M, W, V, R
	U(ph)			Phase	If phase is unstable, then U(ph) gets a value of zero.	M, W, V, F, R
H	H	J	Enthalpy	System		M, W, V, R

V	Abbrev.	Unit	Descript.	Domain	Comment	Suffix
	H(ph)			Phase	If phase is unstable, then H(ph) gets a value of zero.	M, W, V, F
S	S	J/K	Entropy	System		M, W, V, R
	S(ph)			Phase	If the phase is unstable, then S(ph) gets a value of zero.	M, W, V, F, R
Cp	HM.T	J/mol /K	Heat capacity at constant pressure	System	Use only if pressure has been set as a condition.	R
	HM(ph).T			Phase		R
Cv	HM.T	J/mol /K	Heat capacity at constant volume	System	Use only if volume has been set as a condition.	R
	HM(ph).T			Phase		R
D	DG(ph)	N/A	Driving force (thermodynamic factor)	Phase	Already divided by RT.	Always use with M, W, V or F. R can also be used.
Compositional extensive variables (overall amount/size of components in whole system, or amount of a component in system or in a phase)						
n	N	mole	Moles	All components		M, W, V, (R)
	N(comp)			Component		M, W, V, (R)
	N(ph,comp)			Component in a phase		M, W, V, (R)
	NP(ph)			Phase	Not to be used as a condition in POLY. Instead, use CHANGE_STATUS PHASE <PHASE>=FIX <AMOUNT> where the fixed <AMOUNT> is roughly equal to NPF(ph), which cannot be directly evaluated or listed. If the phase is unstable, then NP(ph) and its normalized quantities get zero value.	M, W, V, (R)
b	B	gram	Mass	All components		M, W, V, (R)
	B(comp)			Component		M, W, V, (R)
	B(ph,comp)			Component in a phase		M, W, V, (R)

V	Abbrev.	Unit	Descript.	Domain	Comment	Suffix
	BP(ph)			Phase	Not to be used as a condition in POLY. Instead, use CHANGE_STATUS PHASE <PHASE>=FIX <AMOUNT> where the fixed <AMOUNT> is roughly equal to BPF(ph), which cannot be directly evaluated or listed. If the phase is unstable, then BP(ph) and its normalized quantities get zero value.	M, W, V, (R)
x	X(comp)	N/A	Mole fraction	Component	When plotting this quantity in POST, refer to as "Mole-Fraction <comp>" (abbreviated as "M_F")	(R)
	X(ph,comp)			Component in a phase		(R)
w	W(comp)	N/A	Mass (weight) fraction	Component	When plotting this quantity in POST, refer to as "Weight-Fraction <comp>" (abbreviated as "W_F")	(R)
	W(ph,comp)			Component in a phase		(R)
x %	X%(comp)	N/A	Mole percent	Component	Only available in TQ-Interface and TC-API. Can always be plotted in POST where it is referred to as "Mole-Percent <comp>" (abbreviated as "M_P").	(R)
w %	W%(comp)	N/A	Mass (weight) percent	Component	Only available in TQ-Interface and TC-API. Can always be plotted in POST where it is referred to as "Weight-Percent <comp>" (abbreviated as "W_P").	(R)
u	u-f(ph,comp)	N/A	u-fraction	Component in a stable phase	Cannot be used in POLY, but can be plotted in POST where it is referred to as "u-f".	(R)
in	IN(sp)	mole	Input mole number	Phase species in the system	Only available in TQ-Interface and TC-API.	(R)

V	Abbrev.	Unit	Descript.	Domain	Comment	Suffix
im	IM(sp)	gram	Input mass unit	Phase species in the system	Only available in TQ-Interface and TC-API.	(R)
Constitutional composition-related extensive variables (amount of a constituent/species on a sublattice site in a phase)						
y	Y(ph,cons# sub)	N/A	Site fraction	Constituent on a sublattice site (denoted by # and a digit) in a phase		
Special quantities						
Q	QF(ph)	N/A	Phase stability function	Phase	Negative when phase composition is inside a spinodal, otherwise positive. Can be used to find out if an equilibrium is within the miscibility gap for a solution phase. Cannot be used as a condition.	R Under a condition and system definition, $QFR(ph) = QF(ph)$
Tc	TC(ph)	K	Curie temperature	Phase	Calculated for phases with magnetic contributions in an equilibrium state. Cannot be used as a condition, but can be plotted in POST.	R Under a condition and system definition, $TCR(ph) = TC(ph)$
Mb	BMAG(ph)	N/A	Bohr magneton number	Phase	Calculated for phases with magnetic contributions in an equilibrium state. Cannot be used as a condition, but can be plotted in POST.	R Under a condition and system definition, $BMAGR(ph) = BMAG(ph)$

The u-fraction variable

The u-fraction is an important quantity in some single-point or stepping paraequilibrium calculations in the POLY module and in the DICTRA module. You can apply the variable in a paraequilibrium calculation to the substitutional matrix component, the substitutional alloying components or the interstitial component. The u-fraction is denoted as u_i for the i -th system component n of a whole system or of a specific phase in various equilibrium states (such as full-equilibria, partial-equilibria, para-equilibria, local-equilibria).

Generally, the u-fraction is defined as:

$$\frac{x_i}{\sum_{j \in S} x_j}$$

The sum of x_j in the denominator is calculated for the substitutional matrix element and all substitutional alloying element in the whole system or in a specific phase. The variable x_i in the numerator stands for the mole-fraction of the i -th component in the whole system or in the specific phase.

6.1.2 Suffixes

Suffixes may be appended to all extensive variables and to some intensive variables. Some suffixes can be used to enter the value of variables in normalized form. These are referred to as normalizing suffixes. If the variable that you create with a normalizing suffix is based on a state variable that can be set as a condition in POLY, then the normalized variable can also be set as a condition in POLY.

The normalizing suffixes are M, W, V and F. There is also a reference state suffix "R", which you can use if you want the value of a thermodynamic variable to be calculated with respect to a reference state that have previously set.

Normalizing suffixes

When variables that express system and phase quantities are normalized, the following general rules are used:

- System quantities are normalized by the total system size (in terms of N, B or V).
- Phase quantities are normalized by the phase amount [in terms of NP(ph), BP(ph) or VP(ph)].

The normalized quantities of G(ph), A(ph), U(ph), H(ph), S(ph) and V(ph) are calculated according to the thermodynamic model used for the phase (e.g. GM(ph), AM(ph), UM(ph), HM(ph), SM(ph) and VM(ph)). These quantities are calculated using the first derivatives of the Gibbs energy expressed for the phase with respect to the current composition of the system.

The following table describes the normalizing suffixes for the different state variables.

Suffix	Description	Example(s)
G, A, U, H, S and V of a whole system		
M (per mole)	First derivative of the variable with regard to the total system size in terms of N.	GM is the Gibbs energy per mole of the system (J/mol). $GM = \partial G / \partial N$
W (per mass in gram)	First derivative of the variable with regard to the total system size in terms of B.	GW is the Gibbs energy per mass of the system (J/g). $GW = \partial G / \partial B$
V (per volume in m ³)	First derivative of the variable with regard to the total system size in terms of V. VV does not have to be evaluated.	GV is the Gibbs energy per volume of the system (J/m ³). $GV = \partial G / \partial V$
G(ph), A(ph), U(ph), H(ph), S(ph) and V(ph) of a phase		
M (per mole)	First derivative of the variable with regard to the phase amount in terms of NP(ph).	GM is Gibbs energy of the phase per mole of the phase (J/mol). $GM(ph) = \partial G(ph) / \partial NP(ph)$

Suffix	Description	Example(s)
w (per mass in gram)	First derivative of the variable with regard to the phase amount in terms of BP(ph).	GW is Gibbs energy of the phase per mass of the phase (J/mol). $GW(ph) = \partial G(ph) / \partial BP(ph)$
v (per volume in m ³)	First derivative of the variable with regard to the phase amount in terms of VP(ph). VV(ph) does not have to be evaluated.	GV is Gibbs energy of the phase per volume of the phase (J/mol). $GV(ph) = \partial G(ph) / \partial VP(ph)$
F (per mole formula unit)	First derivative of the variable with regard to the phase amount in terms of NP(ph) and NA (NA is the total atomic number in the phase formula)	GF(ph) is the Gibbs energy of the phase per formula unit of the phase (J/mol). $GF(ph) = \partial G(ph) / \partial NP(ph) * NA$
DG(ph) of a phase		
M (per mole)	Theoretically, the first derivative of the variable with regard to the phase amount in terms of NP(ph). Since DG(ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead. DGM(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.	DGM(ph) is driving force for precipitation of the phase per mole of components. $DGM(ph) = \partial DG(ph) / \partial NP(ph)$
w (per mass in gram)	Theoretically, the first derivative of the variable with regard to the phase amount in terms of BP(ph). Since DG(ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead. DGW(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.	DGW(ph) is driving force for precipitation of the phase per mass of components. $DGW(ph) = \partial DG(ph) / \partial BP(ph)$
v (per volume in m ³)	Theoretically, the first derivative of the variable with regard to the phase amount in terms of VP(ph). Since DG(ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead. DGV(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.	DGV(ph) is driving force for precipitation of the phase per volume of components. $DGV(ph) = \partial DG(ph) / \partial VP(ph)$

Suffix	Description	Example(s)
F (per mole formula unit)	<p>Theoretically, the first derivative of the variable with regard to the phase amount in terms of NP(ph) and NA (NA is the total atomic number in the phase formula). Since DG(ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead.</p> <p>DGF(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.</p>	<p>DGF(ph) is driving force for precipitation of the phase per formula unit of components.</p> $DGF(ph) = \partial DG(ph) / \partial NP(ph) * NA$
N and B of a system		
M (per mole)	<p>First derivative of the variable with regard to the total system size in terms of N.</p> <p>NM does not have to be evaluated.</p> <p>BM cannot be set as a condition.</p>	<p>BM is mass (gram) of components per mole of the system (g/mol).</p> $BM = \partial B / \partial N$
W (per mass in gram)	<p>First derivative of the variable with regard to the total system size in terms of B.</p> <p>BW does not have to be evaluated.</p> <p>NW cannot be set as a condition.</p>	<p>NW is mole number of components per mass of the system (mol/g).</p> $NW = \partial N / \partial B$
V (per volume in m ³)	<p>First derivative of the variable with regard to the total system size in terms of V.</p> <p>BV is the density of the entire system.</p>	<p>NV is mole number of components per volume of the system (mol/m³).</p> $NV = \partial N / \partial V$
N (comp) and B(comp) of a component in the system		
M (per mole)	<p>First derivative of the variable with regard to the total system size in terms of N.</p> <p>BM(c) cannot be set as a condition.</p>	<p>NM(comp) is mole number of a component per mole of the system (mole fraction, that is, X(comp)).</p> $NM(comp) = \partial N(comp) / \partial N$
W (per mass in gram)	<p>First derivative of the variable with regard to the total system size in terms of B.</p> <p>NW(c) cannot be set as a condition.</p>	<p>BW(comp) is mass (gram) of a component per mass of the system (mass fraction, that is, W(comp)).</p> $BW(comp) = \partial B(comp) / \partial B$
V (per volume in m ³)	<p>First derivative of the variable with regard to the total system size in terms of V.</p>	<p>NV(comp) is mole number of a component per volume of the system (mol/m³).</p> $NV(comp) = \partial N(comp) / \partial V$
NP(ph), BP(ph) and VP(ph) of a phase in the system		
M (per mole)	<p>BPM(ph) and VPM(ph): First derivative of the variable with regard to the phase amount in terms of NP(ph).</p> <p>NPM(ph): First derivative of the variable with regard to the total system size in terms of N.</p>	<p>BPM(ph) is mass (gram) of a phase per mole of the phase in the system (g/mol).</p> $BPM(ph) = \partial BP(ph) / \partial NP(ph)$ <p>NPM(ph) is mole number of a phase per mole of the system (mole fraction).</p>

Suffix	Description	Example(s)
		$NPM(ph) = \partial NP(ph) / \partial N$
\bar{w} (per mass in gram)	NPW(ph) and VPW(ph): First derivative of the variable with regard to the phase amount in terms of BP(ph). BPW(ph): First derivative of the variable with regard to the total system size in terms of B.	VPW(ph) is volume (m^3) of a phase per mass of the phase in the system (m^3/g) $VPW(ph) = \partial VP(ph) / \partial BP(ph)$ BPW(ph) is mass (gram) of a phase per mass of the system (mass fraction) $BPW(ph) = \partial BP(ph) / \partial B$
\bar{v} (per volume in m^3)	NPV(ph) and BPV(ph): First derivative of the variable with regard to the phase amount in terms of VP(ph). VPV(ph): First derivative of the variable with regard to the total system size in terms of V.	NPV(ph) is mole number of a phase per volume of the phase in the system (mol/m^3). $NPV(ph) = \partial NP(ph) / \partial VP(ph)$ VPV(ph) is volume (m^3) of a phase per volume of the system (volume fraction). $VPV(ph) = \partial VP(ph) / \partial V$
N(ph,comp) and B(ph,comp) of a component in a phase		
\bar{M} (per mole)	First derivative of the variable with regard to the phase amount in terms of NP(ph) of the phase.	NM(ph,comp) is mole number of a component per mole of a phase (mole fraction of a component in a phase, that is, $X(ph, comp)$). $NM(ph,comp) = \partial N(ph,comp) / \partial NP(ph)$
\bar{w} (per mass in gram)	First derivative of the variable with regard to the phase amount in terms of BP(ph) of the phase.	BW(ph,comp) is mass (gram) of a component per mass of a phase (mass fraction of a component in a phase, that is, $W(ph,comp)$). $BW(ph,comp) = \partial B(ph,comp) / \partial BP(ph)$
\bar{v} (per volume in m^3)	First derivative of variable with regard to the phase amount in terms of VP(ph) of the phase.	NV(ph,comp) is mole number of a component per volume of a phase (mol/m^3). $NV(ph,comp) = \partial N(ph,comp) / \partial VP(ph)$

The reference state suffix R

You can use the reference state suffix “R” for some thermodynamic variables to calculate their value with respect to a reference state that you have previously set for a system component with the SET_REFERENCE_STATE command in POLY (or in a response-driven modules such as the POURBAIX module). The value of energy-related variables that are used with the “R” suffix depends on the reference states of all the components in the defined system. Note that it is possible to use an “R” suffix on all compositional extensive state variables as well, but the value of the state variable will always be the same, with or without the suffix.

If the reference state for a system component is the default reference state (the stable reference state (SER) which is defined in a Thermo-Calc database), then $MUR(comp) = MU(comp)$, $ACR(comp) = AC(comp)$ and $LNACR(comp) = LNAC(comp)$.

In the case of some thermodynamic variables, you can also use the “R” suffix to express chemical potentials and activities of species relative to some single-substitutional-lattice solution phases (such as aqueous solution, gaseous mixture, metallic liquid solution, slag mixture or MO solid solution). These state variables are MU(sp,ph), MUR(sp,ph), AC(sp,ph), ACR(sp,ph), LNAC(sp,ph) and LNACR(sp,ph).

The reference states and standard states of various solution species are pre-defined for some solution phases in some databases. For all solution species in any solution model in any database, it is always the case that MUR(sp,ph)= MU(sp,ph), ACR(sp,ph)= AC(sp,ph) and LNACR(sp,ph)= LNAC(sp,ph).

6.2 Derived variables and partial derivatives

Many derived variables can be obtained easily by using partial derivatives of state variables, such as heat capacity, thermal expansivity, isothermal compressibility, among others.

Derivatives of state variables can be defined or evaluated by putting a dot (“.”) between two state variables. The variable after the dot must be a condition that you have set when you defined your system. For example, the heat capacity (at constant pressure or volume) of a system is the partial derivative of the state variable enthalpy with respect to temperature. To evaluate this derivative, use the designation HM.T, where temperature is a state variable that you have set already.

Any partial derivative of a state variable with respect to another can be defined or evaluated as a derived variable by using the dot “.” notation. The following table shows some examples:

Derived variable	Description
HM.T = $\partial \text{HM} / \partial T$	Heat capacity for the system at either constant P if pressure is a condition or constant V if volume is a condition.
HM(ph).T = $\partial \text{HM}(\text{ph}) / \partial T$	Heat capacity for a phase at either constant P if pressure is a condition or constant V if volume is a condition.
H.T = $\partial H / \partial T$	Heat capacity for the system multiplied by total mole number of components, i.e., $\partial H / \partial T = C_p * N$ if pressure is a condition in a closed system or $\partial H / \partial T = C_v * N$ if volume is a condition in a closed system.
H(ph).T = $\partial H(\text{ph}) / \partial T$	Heat capacity for a phase multiplied by the sum of NP(ph) and HM(ph)* $\partial \text{NP}(\text{ph}) / \partial T$, i.e., $C_p(\text{ph}) * \text{NP}(\text{ph}) + \text{HM}(\text{ph}) * \partial \text{NP}(\text{ph}) / \partial T$ if pressure is a condition or $C_v(\text{ph}) * \text{NP}(\text{ph}) + \text{HM}(\text{ph}) * \partial \text{NP}(\text{ph}) / \partial T$ if volume is a condition.
VM.T = $\partial \text{VM} / \partial T$	Thermal expansivity of the system (already multiplied by the total molar volume), i.e., $\partial \text{VM} / \partial T = \alpha * \text{VM}$.
VM(ph).T = $\partial \text{VM}(\text{ph}) / \partial T$	Thermal expansivity of a phase (already multiplied by its molar volume), i.e., $\partial \text{VM}(\text{ph}) / \partial T = \alpha(\text{ph}) * \text{VM}(\text{ph})$.
V.T = $\partial V / \partial T$	Thermal expansivity of the system (already multiplied by the total volume), i.e., $\partial V / \partial T = \alpha * V$.
V(ph).T = $\partial V(\text{ph}) / \partial T$	Thermal expansivity of a phase (already multiplied by the phase volume) plus the VM(ph)* $\partial \text{NP}(\text{ph}) / \partial T$ term, i.e., $\partial V(\text{ph}) / \partial T = \alpha(\text{ph}) * V(\text{ph}) = \alpha(\text{ph}) * \text{VM}(\text{ph}) * \text{NP}(\text{ph}) + \text{VM}(\text{ph}) * \partial \text{NP}(\text{ph}) / \partial T$.

Derived variable	Description
$VM.P = -\partial VM / \partial P$	Isothermal compressibility of the system (already multiplied by the total molar volume), i.e., $\partial VM / \partial P = -\kappa * VM$.
$VM(ph).P = -\partial VM(ph) / \partial P$	Isothermal compressibility of a phase (already multiplied by its molar volume), i.e., $\partial VM(ph) / \partial P = -\kappa(ph) * VM(ph)$.
$V.P = -\partial V / \partial P$	Isothermal compressibility of the system (already multiplied by the total volume), i.e., $\partial V / \partial P = -\kappa * V$.
$V(ph).P = -\partial V(ph) / \partial P$	Isothermal compressibility of a phase (already multiplied by the phase volume) plus the $VM(ph) * \partial NP(ph) / \partial P$ term, i.e., $\partial V(ph) / \partial P = -\kappa(ph) * V(ph) = -\kappa(ph) * VM(ph) * NP(ph) + VM(ph) * \partial NP(ph) / \partial P$.
$T.X(comp) = \partial T / \partial X(comp)$	Slope of a phase boundary on a T-X(comp) phase diagram with respect to mole fraction of the component in the system.
$T.W(comp) = \partial T / \partial W(comp)$	Slope of a phase boundary on a T-W(comp) phase diagram with respect to mass of the component in the system.
$T.X(ph,comp) = \partial T / \partial X(ph,comp)$	Slope of a phase boundary on a T-X(ph,comp) phase diagram with respect to mole fraction of the component in the phase.
$T.W(ph,comp) = \partial T / \partial W(ph,comp)$	Slope of a phase boundary on a T-W(ph,comp) phase diagram with respect to mole fraction of the component in the phase.
$P.T = \partial P / \partial T$	Slope of a phase boundary on a P-T phase diagram (Note that the equilibrium with phase assemblage must be calculated first).

6.2.1 Defining new derived variables and functions

You can define additional derived variables or functions based on a state variable by using the ENTER_SYMBOL command. Any derived variable or function must have a unique name that starts with a letter and has a maximum number of eight characters. These characters can include both uppercase and lowercase letters, numerical digits and the underscore character ("_"). No other characters are allowed.

The difference between new derived variables introduced with the ENTER_SYMBOL command and new functions introduced with the same command is the following: Whenever Thermo-Calc calculates the value of a function (as part of an equilibrium calculation for example), all functions related to the defined system will be evaluated. A derived variable that you have entered, on the other hand, is only evaluated when it is defined and when it is re-evaluated with the EVALUATE_FUNCTIONS command.

6.2.2 Derived variables for aqueous solutions

Standard state variables used for other phases can be directly applied to the aqueous solution phase. In addition, there are pre-defined derived variables for the aqueous solution phase in particular. Examples of predefined derived variables for the aqueous solution phase are listed and briefly described in the following table. Some derived variables for a gaseous mixture phase are also listed in the table. This is because EOS (Equation of State) expressions, standard thermodynamic properties and transport properties of the pure solvent H₂O are also expressions and properties of the pure gaseous species H₂O.

Name	Abbrev.	Units	Description	Comments
For Aqueous Solution Phase				
pH	PH	N/A	Acidity	of the aqueous solution phase $\text{pH} = -\log_{10}(\text{AC}(\text{H}^+)) = -\log_{10}(\text{ACR}(\text{H}^+, \text{AQ}))$
Eh	EH	V, mV	Hypothetical electric potential	of the aqueous solution phase $\text{Eh} = u(\text{ZE})/96485.309$
Pe	PE	N/A	Logarithm of the hypothetical electron activity	of the aqueous solution phase $\text{pe} = u(\text{ZE})/(2.3025851 * \text{RT})$
Ah	AH	kJ, kcal	Thermodynamic affinity per electron	of a redox couple wrt the standard hydrogen electrode in the aqueous solution phase $\text{Ah} = u(\text{ZE})$
yw	YH2O	N/A	Mole fraction	of the solvent H2O in the aqueous solution phase $\text{YH2O} = \text{Y}(\text{AQ}, \text{H2O})$
Nw	AH2O	mole	Mole number	of 1.0 kg of solvent H2O $\text{AH2O} = 55.508435$
Nsp	NSH2O	mole	Mole number, NS(AQ,H2O)	of the solvent (H2O) in the aqueous solution phase $\text{NS}(\text{AQ}, \text{H2O}) = \text{YH2O} * \text{NP}(\text{AQ})$
	NS#		Mole number, NS(AQ,sp)	of a solute species in the aqueous solution phase $\text{NS}(\text{AQ}, \text{sp}) = \text{Y}(\text{AQ}, \text{sp}) * \text{NP}(\text{AQ})$
M	ML#	mol/kg_H2O	Molality, ML(AQ,sp)	of a solute species in the aqueous phase $\text{ML}(\text{AQ}, \text{sp}) = \text{Y}(\text{AQ}, \text{sp}) * \text{AH2O} / \text{YH2O}$
m*	TIM	equivalent molality	Total molality	of all solute species in the aqueous solution phase $\text{TIM} = \text{sum}[\text{ML}(\text{AQ}, \text{sp})]_{\text{ions}} + \text{sum}[\text{ML}(\text{AQ}, \text{sp})]_{\text{complexes}}$
mt	TIC#	equivalent molality	Total ionic concentration, TIC(AQ,sp)	of a cation I in the aqueous phase $\text{TIC}(\text{AQ}, \text{spI}) = \text{sum}[\text{ML}(\text{AQ}, \text{sp}) * V(\text{spI} - \text{in-spI})]$
I	ISTR	N/A	Ionic strength	of the aqueous solution phase $\text{ISTR} = 1/2 * \text{sum}[\text{ML}(\text{AQ}, \text{sp}) * Z(\text{AQ}, \text{sp})^2]$
γ	RCH2O	N/A	Activity coefficient, RC(H2O,AQ)	of the solvent (H2O) $\text{RC}(\text{H2O}, \text{AQ}) = \text{ACR}(\text{H2O}, \text{AQ}) / \text{YH2O}$
	RC#		Activity coefficient, RC(sp,AQ)	of a solute species $\text{RC}(\text{sp}, \text{AQ}) = \text{ACR}(\text{sp}, \text{AQ}) / \text{Y}(\text{AQ}, \text{sp}) * \text{YH2O}$
α i	AIH2O	N/A	Activity, AI(H2O,AQ)	of the solvent (H2O), $\text{AI}(\text{H2O}, \text{AQ}) = \text{ACR}(\text{H2O}, \text{AQ})$
	AI#		Activity, AI(sp,AQ)	of a solute species related to the aqueous solution phase, $\text{AI}(\text{sp}, \text{AQ}) = \text{ACR}(\text{sp}, \text{AQ}) * \text{AH2O}$

	LogAI#		Log10 Activity, LogAI(H2O,AQ), LogAI(sp,AQ)	of the solvent or a solute species related to the aqueous solution phase in common logarithm, $\text{LogAI(H2O,AQ)} = \log_{10}[\text{AI(H2O,AQ)}]$ $\text{LogAI(sp,AQ)} = \log_{10}[\text{AI(sp,AQ)}]$
α_w	AW	N/A	Activity	of H2O in the aqueous solution phase $\text{AW} = \text{ACR(H2O,AQ)}$
ϕ	OS	N/A	Osmotic coefficient	of aqueous solution phase $\text{OS} = -55.508435 \cdot \ln \text{AW} / \text{TIM}$
At1	AT1	equil_mol/kg_H2O	Titration alkalinity (definition 1)	of the aqueous solution phase Generally defined as the equivalent molality of carbonate and bicarbonate at the methyl orange endpoint (pH=4.5).
At2	AT2	equil_mol/kg_H2O	Titration alkalinity (definition 2)	of the aqueous solution phase Generally defined as the equivalent molality of carbonate and bicarbonate, plus sulfide, at the methyl orange endpoint (pH=4.5).
For Gaseous Mixture Phase				
γ	RA#	N/A	Activity coefficient, RA(sp,GAS)	of a gaseous species in the gaseous mixture $\text{RA(sp,GAS)} = \text{function(Y,T,P)}$
γ^*	RF#	N/A	Fugacity coefficient, RF(sp,GAS)	of a pure gaseous species under TP $\text{RF(sp,GAS)} = \text{function(T,P/V)}$
F	FUG#	pa, bar, psi	Fugacity, FUG(sp,GAS)	of a gaseous species in the gaseous mixture $\text{FUG(sp,GAS)} = \text{RA(sp,GAS)} \cdot \text{RF(sp,GAS)} \cdot \text{Y(GAS,sp)} \cdot \text{P}$
ft	TFUG	pa, bar, psi	Total gas fugacity	of the gaseous mixture phase $\text{TFUG} = \text{sum}[\text{FUG(sp,GAS)}]$

Defining new derived variables for aqueous solutions

You can define many different additional derived variables and functions. For instance, the partition coefficient of a component between two phases is defined as follows:

$$\text{Pc<name>} = \text{X(phase1,component)} / \text{X(phase2,component)}$$

Another example is the activity coefficient of a component in the system. It is defined as follows:

$$\text{Rc<name>} = \text{ACR(component)} / \text{X(component)}$$

The activity coefficient of a species in a solution phase depends on which model definitions on the reference states that are used and it depends on the standard states for the species. If the standard state of a species is defined to be the same as the “pure species” in a substitutional phase, then the activity coefficient of the species can be calculated as:

$$RC<name> = ACR(species,phase)/Y(phase,species)$$

In some cases, there are more than one sublattice in the phase and the reference states for the phase species cannot be presented by the “pure species”, as in the case of C in FCC $[(Fe)_1(C,N,VA)_1]$, where the model may end at fifty percent C and fifty percent Fe. In those cases, the chemical potential and activity of all phase constituents will not be well defined and you will not be able to properly define the activity coefficients of the species in the phase.

For an aqueous solution phase, no matter what model is used, the reference state and standard state for both the solvent and solutes are defined in a special way in the Thermo-Calc software. The reference state for the solvent is set as “pure water”, the same as its standard state (according to Raoult's Law). The standard state for a solute species is set the “hypothetical solute species”, whilst its reference state is defined as the “hypothetical state at unit molality (one mole dissolved into 1.0 kg of solvent) but in which the environment of each molecular is the same as at infinite dilution” (according to Henry's Law). Under these definitions, the activity coefficients for solvent species can be calculated as follows:

$$RC<H2O> = ACR(H2O,aqueous)/Y(aqueous,H2O)$$

The coefficients for the solute species can be calculated as follows:

$$\begin{aligned} RC<spec> &= AI(species,aqueous)/ML(aqueous,species) \\ &= ACR(species,aqueous)/Y(aqueous,species)*Y(aqueous,H2O) \end{aligned}$$

AI is here the activity of solute species calculated from the model, and ML is the molality of the species.

6.2.3 Thermodynamic variables and wildcard characters

The ACR(species,phase) and the MUR(species,phase) quantities can only be appropriately and meaningfully applied to substitutional solution phases (such as GAS, AQUEOUS, LIQUID) and to solution phases without an interstitial sublattice set. This means that the wild card characters “*” and “\$” normally don't work properly for the activity and/or chemical potential properties. For examples, you should not use ACR(*,*) or MUR(*,*) for all the species relative to all phases, nor ACR(*,phase) or MUR(*,phase) for all the species relative to a specific phase, nor ACR(species,*) or MUR(species,*) for a specific species relative to all phases.

Instead, use specific names for species and (applicable) phase, as in the following examples:

SHOW_VALUE ACR(Fe+2,AQUEOUS)	Lists activity of the Fe+2 species in AQUEOUS solution phase
SHOW_VALUE MUR(C2,GAS)	Lists chemical potential of the C2 species in GAS mixture phase
SET_AXIS_VAR Y AC(O2,GAS)	Sets activity of the O2 species in GAS mixture phase as Y-axis

6.3 Units of State Variables and Derived Variables

The units for the state variables in the “Units” column in the table in section 6.1.1 are the SI units that are used in the POLY module. However, in the POST module, you can both use pre-defined symbols and define your own symbols which are based on state variables and derived variables. By doing this, you can express the value of the thermodynamic variables listed in section 6.1.1 in non-default units. The following section briefly describes how you can create your own symbols and suggests expressions that you can use to convert default units into other standard units which are not default units in Thermo-Calc.

Section 6.3.2 describes some variables of specific species in a phase and the units in which they are expressed. These variables are not used in POLY or POST, but in the GIBBS, DATA, PARROT and ED_EXP modules.

6.3.1 User-specified units

You need not always use the default units for various variables. With the ENTER_SYMBOL command, you can convert the value of variable from the default unit to your preferred unit. (Some response-driven modules also allow you to set conditions in non-default units.) User-defined symbols in the form of functions can be used for plotting in the POST module, but they cannot be used as conditions in POLY. User defined symbols in the form of variables can be used as conditions.

For example, if you want pressure to be plotted in bar rather than Pa, then you could define the following function “PB”:

```
ENTER_SYMBOL FUNCTION PB = P/1E5 ;
```

If you wanted heat capacity of a system to be shown as in terms of J/mol/K, then you could define the following function Cp:

```
ENTER_SYMBOL FUNCTION Cp = Hm.T ;
```

If the variable you want to convert is a function of one or more derivatives, then you must enter the symbol as a variable rather as a function. For instance, a symbol expressing heat capacity of a system in a unit of cal/mol/K could be defined as the following variable “Cp2”:

```
ENTER_SYMBOL VARIABLE Cp2 = Hm.T/4.1858 ;
```

See the entry about ENTER_SYMBOL in the *Thermo-Calc Console Mode Command Reference* for more information about this command.

Given on the following pages are just a few of suggested examples for entering such conventional functions and their associated units in various possible ways.

Examples of possible user-defined units

The following table presents examples of expressions that you can use to enter symbols that allow you to present the values of thermodynamic variables in a variety of units.

Note that you for can also use thermodynamic variables with normalizing suffixes in the expression when you enter a symbol. However, the table below does not contain any examples of such expressions.

In the expressions, “i” stands for an auxiliary index or letter that corresponds to the component “c”, “j” stands for an auxiliary index or letter that corresponds to the phase “ph”, and “ij” stands for an auxiliary index or letter that corresponds to the component “c” in the phase “ph”.

Quantity	Suggested name and expression	Unit
For intensive variables of a defined system		
Temperature	TempC = T-273.15	Celsius (C)
	TempF = 1.8*T-459.67	Fahrenheit (F)
	TempF = 1.8*TempC+32	
Pressure	PB = P/1E5	bars (bar)
	PKb = P/1E8	kilobars (kbar)
	PAtm = P/101325	atmosphere (atm)
	PSI = P/6894.76	pounds/sq. inch (psi)
	PIHg = P/3342.11	inches of Hg
	PTor = P/133.322	Tors (millimeters of Hg)
For extensive variables of a defined system		
Amount	BKg = 1E-3*B	kilograms (kg)
	BTon = 1E-6*B	tons
Volume	VDM = 1E-3*V	cubic decimeters (dm3, l)
	VCM = 1E-6*V	cubic centimeters (cm3)
	VMM = 1E-9*V	cubic millimeters (mm3)
	VCI = 1.6387064E-5*V	cubic inches (in3)
	VLi = 1E-3*V	liters (l)
Energy	GCal = G/4.1858	cal
	ACal = A/4.1858	cal
	UCal = U/4.1858	cal
	HCal = H/4.1858	cal
	SCal = S/4.1858	Cal/K
Heat Capacity	Cp2 = HM.T/4.1858	cal/mol/K
	Cp3 = HW.T/4.1858	cal/g/K
	Cp4 = HV.T/4.1858	cal/m3/K
Thermal Expansion	A2 = VM.T*1E-6*VM	cm3/mol/K
	A3 = VW.T*1E-6*VM	cm3/g/K
Isothermal Compressibility	B2 = -VM.P*1E-9*VM	mm3/mol/Pa
	B3 = -VW.P*1E-9*VM	mm3/g/Pa
For intensive variables of a system component		
Chemical Potential	MUi = MU(c)/4.1858	cal/mol
	MURi = MUR(c)/4.1858	cal/mol
Special quantity for aqueous solution	pH = -LOG10(ACR(H+1))	dimensionless
	Eh = MUR(ZE)/RNF where RNF=96485.309	volts (V)
For extensive variables of a system component		
Amount	MFi = N(c)/N = X(c)	dimensionless
	MPi = N(c)/N*100	dimensionless
	WFi = B(c)/B = W(c)	dimensionless
	WPi = B(c)/B*100	dimensionless

	$BK_{gi} = 1E-3 \cdot B(c)$	kilograms (kg)
	$BT_{oni} = 1E-6 \cdot B(c)$	tons
For extensive variables of a phase		
Amount	$MF_j = NP(ph)/N$	dimensionless
	$MP_j = NP(ph)/N \cdot 100$	dimensionless
	$WF_j = BP(ph)/B$	dimensionless
	$WP_j = BP(ph)/B \cdot 100$	dimensionless
	$BK_{gj} = 1E-3 \cdot BP(ph)$	kilograms (kg)
	$BT_{onj} = 1E-6 \cdot BP(ph)$	tons
Volume	$VCM_j = 1E-3 \cdot V(ph)$	cubic decimeters (dm ³ , l)
	$VCM_j = 1E-6 \cdot V(ph)$	cubic centimeters (cm ³)
	$VMM_j = 1E-9 \cdot V(ph)$	cubic millimeters (mm ³)
Energy	$GCal_j = G(ph)/4.1858$	cal
	$ACal_j = A(ph)/4.1858$	cal
	$UCal_j = U(ph)/4.1858$	cal
	$HCal_j = H(ph)/4.1858$	cal
	$SCal_j = S(ph)/4.1858$	Cal/K
Driving Force	$DG2_j = DGM(ph)/4.1858$	cal/mol
	$DG3_j = DGW(ph)/4.1858$	cal/g
	$DG4_j = DGV(ph)/4.1858$	Cal/m ³
	$DG5_j = DGF(ph)/4.1858$	cal/mole_formula_unit
Heat Capacity	$Cp2_j = HM(ph) \cdot T/4.1858$	cal/mol/K
	$Cp3_j = HW(ph) \cdot T/4.1858$	cal/g/K
	$Cp4_j = HV(ph) \cdot T/4.1858$	cal/m ³ /K
	$Cp5_j = HF(ph) \cdot T/4.1858$	cal/mole_formula_unit/K
Thermal Expansion	$A2_j = VM(ph) \cdot T \cdot 1E-6 \cdot VM$	cm ³ /mol/K
	$A3_j = VW(ph) \cdot T \cdot 1E-6 \cdot VM$	cm ³ /g/K
	$A4_j = VF(ph) \cdot T \cdot 1E-6 \cdot VM$	cm ³ /mole_formula_unit/K
Isothermal Compressibility	$B2_j = -VM(ph) \cdot P \cdot 1E-9 \cdot VM$	mm ³ /mol/Pa
	$B3_j = -VW(ph) \cdot P \cdot 1E-9 \cdot VM$	mm ³ /g/Pa
	$B4_j = -VF(ph) \cdot P \cdot 1E-9 \cdot VM$	mm ³ /mole_formula_unit/Pa
For extensive variables of a component in a phase		
Amount	$MF_{ij} = N(ph,c)/NP(ph) = X(ph,c)$	dimensionless
	$MP_{ij} = N(ph,c)/NP(ph) \cdot 100$	dimensionless
	$WF_i = B(ph,c)/BP(ph) = W(ph,c)$	dimensionless
	$WP_{ij} = B(ph,c)/BP(ph) \cdot 100$	dimensionless
	$BK_{gij} = 1E-3 \cdot B(ph,c)$	kilograms (kg)
	$BT_{onij} = 1E-6 \cdot B(ph,c)$	tons
For intensive variables of a species in a phase		
Chemical Potential	$MUCal_{ij} = MU(sp,ph)/4.1858$	cal/mol
	$MUErg_{ij} = MU(sp,ph) \cdot 1E7$	cal/mol
Fugacity	$FA_{ij} = AC(sp,ph) \cdot PATM$	atmosphere (atm)
	$FB_{ij} = AC(sp,ph) \cdot PB$	bars (bar)
	$FC_{ij} = AC(sp,ph) \cdot PKB$	kilobars (kbar)
	$FT_{ij} = AC(sp,ph) \cdot PTOR$	Tors (millimeters of Hg)
ln(Fugacity)	$LnFA_{ij} = LNAC(sp,ph) + LN(PATM)$	atmosphere (atm)
	$LnFB_{ij} = LNAC(sp,ph) + LN(PB)$	bars (bar)

	$\text{LnFCij} = \text{LNAC}(\text{sp}, \text{ph}) + \text{LN}(\text{PKB})$	kilobars (kbar)
	$\text{LnFTij} = \text{LNAC}(\text{sp}, \text{ph}) + \text{LN}(\text{PTOR})$	Tors (millimeters of Hg)
Special quantity for aqueous solution	$\text{Alij} = \text{ACR}(\text{FE}+3, \text{AQ}) * \text{AH2O}$	dimensionless
	$\text{RCij} = \text{ACR}(\text{FE}+3, \text{AQ}) * \text{YH2O} / \text{Y}(\text{AQ}, \text{FE}+3)$ where $\text{AH2O} = 55.508435$ and $\text{YH2O} = \text{Y}(\text{AQ}, \text{H2O})$	dimensionless
	$\text{WRCalij} = \text{WR}(\text{AQ}, \text{sp}) / 4.1858$ ($\text{WR}(\text{AQ}, \text{sp})$ is only valid for aqueous species in a system in which the AQUEOUS solution phase is considered)	cal/mol
For extensive variables of a species in a phase		
Special quantity for aqueous solution	$\text{MLij} = \text{Y}(\text{AQ}, \text{FE}+3) * \text{AH2O} / \text{YH2O}$	molality (m)
	$\text{ISTR} = 1 * \text{IS1} + 1 * \text{IS2} + 1 * \text{IS3}$ where $\text{AH2O} = 55.508435$, $\text{YH2O} = \text{Y}(\text{AQ}, \text{H2O})$ and $\text{ISn} = .5 * \text{MLi} * \text{Zi}^{**2} + .5 * \text{MLj} * \text{Zj}^{**2} + .5 * \text{MLk} * \text{Zk}^{**2}$	molality (m)

6.3.2 Units for variables of specific species in a phase

In the GIBBS, DATA, PARROT and ED_EXP modules, there are quantities that describe various thermodynamic, physical, chemical and transport properties for a compound phase, and for a certain species or a given species combination in a specific solution phase. The following table describes the units for those variables. Note that these variables cannot be directly used in the POLY module, nor in the POST module

Variables	Description and unit
G(ph,sp) G(ph,sp;0) G(ph,sp1;sp2;...;0)	Gibbs energy (J/mol) of a pure substance or end-member.
G(ph,sp1,sp2,...) L(ph,sp1,sp2,...) G(ph,sp1,sp2,...;0) L(ph,sp1,sp2,...;0) G(ph,sp1,sp2,...;...;0) L(ph,sp1,sp2,...;...;0)	Zero-order interaction parameter (J/mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
G(ph,sp1,sp2,...;i) L(ph,sp1,sp2,...;i) G(ph,sp1,sp2,...;...;i) L(ph,sp1,sp2,...;...;i)	The ith-order interaction parameter (J/mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
TC(ph,sp) TC(ph,sp;0) TC(ph,sp1;sp2;...;0)	Curie temperature (K) of a pure substance or end-member.
TC(ph,sp1,sp2,...) TC(ph,sp1,sp2,...;0) TC(ph,sp1,sp2,...;...;0)	Zero-order Curie-temperature contribution (K) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
TC(ph,sp1,sp2,...;i) TC(ph,sp1,sp2,...;...;i)	The ith-order Curie-temperature contribution (K) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
BMAGN(ph,sp) BMAGN(ph,sp;0)	Bohr magneton number (dimensionless) of a pure substance or end-member.

BMAGN(ph,sp1;sp2,...;0)	
BMAGN(ph,sp1,sp2,...) BMAGN (ph,sp1,sp2,...;0) BMAGN (ph,...;sp1,sp2,...;0)	Zero-order Bohr magneton number (dimensionless) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
BMAGN(ph,sp1,sp2,...;i) BMAGN(ph,sp1,sp2,...;...;i)	The ith-order Bohr magneton number (dimensionless) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
V0(ph,sp) V0(ph,sp;0) V0(ph,sp1;sp2,...;0)	Molar volume (m ³) at 1 bar and reference T0 of a pure substance or end-member.
V0(ph,sp1,sp2,...) V0(ph,sp1,sp2,...;0) V0(ph,sp1,sp2,...;...;0)	Zero-order composition-dependent molar volume (m ³) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
V0(ph,sp1,sp2,...;i) V0(ph,sp1,sp2,...;...;i)	The ith-order composition-dependent molar volume (m ³) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VA(ph,sp) VA(ph,sp;0) VA(ph,sp1;sp2,...;0)	Integrated thermal expansivity (m ³ /mol/K) of a pure substance or end-member.
VA(ph,sp1,sp2,...) VA(ph,sp1,sp2,...;0) VA(ph,sp1,sp2,...;...;0)	Zero-order composition-dependent thermal expansivity (m ³ /mol/K) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VA(ph,sp1,sp2,...;i) VA(ph,sp1,sp2,...;...;i)	The ith-order composition-dependent thermal expansivity (m ³ /mol/K) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VC(ph,sp) VB(ph,sp;0) VB(ph,sp1;sp2,...;0)	Isothermal compressibility (m ³ /mol/Pa) of a pure substance or end-member.
VC(ph,sp1,sp2,...) VB(ph,sp1,sp2,...;0) VB(ph,sp1,sp2,...;...;0)	Zero-order composition-dependent isothermal compressibility (m ³ /mol/Pa) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VC(ph,sp1,sp2,...;i) VB(ph,sp1,sp2,...;...;i)	The ith-order composition-dependent isothermal compressibility (m ³ /mol/Pa) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VK(ph,sp) VB(ph,sp;0) VB(ph,sp1;sp2,...;0)	High-pressure fitting parameter (m ³ /mol) of a pure substance or end-member.
VK(ph,sp1,sp2,...) VB(ph,sp1,sp2,...;0) VB(ph,sp1,sp2,...;...;0)	Zero-order composition-dependent high-pressure fitting parameter (m ³ /mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.

VK(ph,sp1,sp2,...;i) VB(ph,sp1,sp2,...;i)	The ith-order composition-dependent high-pressure fitting parameter (m ³ /mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
WR(ph,sp) WR(ph,sp;0)	Standard Born function (J/mol) of a specific aqueous species in the AQUEOUS solution phase (always with a single sublattice) under the reference-state temperature and pressure.

7 Appendix 2 – List of examples in the Thermo-Calc Console Examples Collection

#	Description
1	Calculation of the binary Fe-C phase diagram (Exploring the HELP facilities).
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 Fe-Cr phase diagram (How to handle miscibility gap).
5	Calculation of a vertical section in the Al-Mg-Si system.
6	Calculation of an isopleth in low alloyed Fe-Mn-Si-Cr-Ni-C steel.
7	Calculation of single equilibria in low alloyed Fe-Mn-Si-Cr-Ni-C steel.
8	Calculation of property diagrams for a high speed steel.
9	Calculation of Dew Point.
10	Preventing clogging of Cr ₂ O ₃ in a continuous casting process.
11	Oxidation of Cu ₂ S with H ₂ O/O ₂ gas.
12	Tabulation of thermodynamic data for reactions.
13	Calculation of phase diagram and G curve using the BINARY module.
14	Calculation of heat and heat capacity variations during solidification of an Al-Mg-Si alloy.
15	Solidification simulation of a Cr-Ni alloy using the SCHEIL module.
16	Calculation of the second order transition line in the Bcc field of the Al-Fe system.
17	Calculation of pseudo-binary phase diagram in the CaO-SiO ₂ system.
18	Calculation of the A ₃ temperature of a steel and the influence of each alloying element on this temperature.
19	Mapping of univariant equilibria with the liquid in Al-Cu-Si. Part A. Step-by-step calculation using POLY. Part B. Calculation made using TERNARY module.
20	Calculation of adiabatic decompression in a geological system.
21	Demonstrates the use of a user-defined database.
22	Calculation of heat balance.
23	Calculation of a para-equilibrium and the T ₀ temperature.
24	Simulation of the silicon arc furnace using the REACTOR module.
25	Simulation of steel refining.
26	Plotting of the partial pressure of gas species along the solubility lines in the As-Ga Phase diagram.
27	CVD calculations.
28	Calculation of PRE.
29	Calculation of speciation of a gas.

30	Scheil solidification simulation for Al-4Mg-2Si-2Cu alloy. Part A. Step-by-step calculation using POLY. Part B. Simulation performed using SCHEIL
31	CVM calculation.
32	Calculation of oxide layers on steel.
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.
35	Calculation of potential diagram.
36	Assessment - The use of the PARROT module.
37	Calculation of an isothermal section using command lines.
38	Calculation of the Morral "rose".
39	Calculation of the reversible Carnot cycle of a heat engine.
40	POURBAIX module.
41	Calculation of a solubility product.
42	Formation of Para-pearlite (Isopleth calculation).
43	Formation of Para-pearlite (Calculation of Isothermal Section).
44	Exploring the usage of variables and functions.
45	3D-diagram with the gamma volume in the Fe-Cr-C system.
46	3D-diagram with the liquidus surface of the Fe-Cr-C system.
47	Quarternary diagram with the gamma volume in the Fe-Cr-V-C system at 1373K.
48	Scheil Simulation with Interstitial Back Diffusion.
49	Quasichemical Model via G-E-S.
50	Quasichemical Model via TDB.
51	Calculation of molar volume, thermal expansivity and density.
52	Changing the excess models for interaction parameters in a solution phase.
53	Pourbaix Diagram Calculations through the TDB-GES-POLY-POST routine.