

Thermo-Calc Graphical Mode User Guide

Version 2015a



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1. Introduction

This guide is for new users of Thermo-Calc who want to work in Graphical Mode. This guide includes an overview of the software and its underlying structure, describes the GUI, how to define a system of components, set up and run calculations, and visualise the results. A basic understanding of thermodynamics is required.

1.1 The Thermo-Calc software program

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, property grids and phase diagrams. A property grid shows how a property—such as the amount of a certain phase for example—varies along two dimensions—the compositions of two components for example.

The program supports stoichiometric and non-ideal solution models and databases. These models and databases are used to make calculations on a variety of materials such as steels, alloys, slags, salts, ceramics, solders, polymers, subcritical aqueous solutions, supercritical electrolyte solutions, non-ideal gases and hydrothermal fluids or organic substances. The calculations take into account a wide ranges of temperature, pressure and composition conditions—the temperature can be set up to 6000 K and pressure up to 1 Mbar.

There are two interfaces available with the Thermo-Calc program, the *Console Mode*, which uses a command line interface, and the *Graphical Mode*, which is the graphical user interface (GUI) version described in this guide.

1.2 Learning Resources



Additional documentation is available on Thermo-Calc Software's website http://www.thermocalc.com/support/documentation/.

There is also online help available that contains general information about the Graphical Mode, information about most **Configuration** window settings, as well as descriptions of two step-by-step examples.

You can access online help information in several ways:

- Select Help > Help Contents to open a list of online help contents in your default web browser. Click Graphical Mode to get access to all the help pages that are available in the GUI.
- In one of the main windows of the Graphical Mode GUI, the **Configuration** window, you can click the help button (2) to view help information regarding the tab that is currently shown in this window. The help information is shown in the default web browser.

Example Collections

To learn more about how to use Thermo-Calc, you can open and run the example projects in the *Thermo-Calc Graphical Examples Collection*. These are in the format of Thermo-Calc project files (*.TCU).

The examples are the following:

- Calculating a single-point equilibrium
- Stepping in temperature in the Fe-C system
- The Fe-C phase diagram



- Ternary phase diagram in the Fe-Cr-C system at 1000 K
- The stable and the metastable Fe-C phase diagrams
- Serially coupled equilibrium calculators
- User defined functions
- Scheil and equilibrium solidification

1.3 Typographical Conventions

The following conventions are used:

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

1.4 Software program overview

The Thermo-Calc software architecture consists of modules that handle, for example, database retrieval and management, calculation, visualisation and diagram plotting. See the <u>Thermo-Calc</u> <u>Console Mode User Guide</u> for more information about the modular architecture of the software.

Most of the calculation types done in the Console Mode can also be performed in Graphical Mode. However, you can only do data optimisation and thermodynamic or kinetic assessments in the Console Mode.

The two modes can be run simultaneously, but there is no communication between them. What you do in the Graphical Mode does not affect the state of the Console Mode session and vice versa. There is one exception to this. The options you set for plotting in the **Results** window or the **Console Results** window are applied to how diagrams are plotted in both modes.

In the Thermo-Calc Graphical Mode, calculations are always set up, carried out, and visualised as part of a project. These different steps in your project is performed by different types of activities.

2. The Graphical Mode interface

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

2.1 The layout

Figure 1 is an example of the default layout of the windows in Graphical Mode. You can easily reorganize the windows yourself. See <u>Moving windows</u>.





Figure 1 The Graphical Mode default window layout.

The windows in Figure 1 are:

- 1. **Project**: Create, manipulate and navigate between the activities that make up a project.
- 2. **Configuration**: Shows the settings that can be configured for the currently selected activity.
- 3. **Scheduler**: Displays information about jobs, such as calculations, that are being performed or that are scheduled to be performed. You can cancel scheduled jobs and if a job has failed, then you can view information about the error.
- 4. **Event Log**: By default this window is closed, but it opens when a calculation is run to show detailed progress information.
- 5. **Results**: Shows the results of a calculation, either plotted as a diagram or displayed in table format.

2.2 Project activities and the tree structure

2.2.1 The tree structure

In a project, a set of linked activities (see <u>Project activity nodes</u>) is called a *tree*. A result calculated within a tree is fed as input into the next activity in the tree. Consequently, if you have an Equilibrium Calculator with another Equilibrium Calculator as its successor, the successor takes the calculation results of the predecessor as the starting values for its calculation. See <u>Successor and predecessor nodes</u> for more information.



The Project window in Figure 2 shows a project with two trees. Within each tree, settings and calculation results are propagated downward until the calculation and the visualisation of the results are completed. However, the system definitions, settings and calculation results of the two trees are independent of each other.



Figure 2 An example of a project with two trees with successor and predecessor activity nodes.

2.2.2 Project activity nodes

Table 1 is a brief description of the project activity types. When working with activities in the Project window these are also referred to as *nodes* in the tree structure.

Table	1	Project	activity	types.
-------	---	---------	----------	--------

Activity type	Description
System Definer	The System Definer activity is used to define a certain thermodynamic system and to read it from file into memory. Also see <u>System definer</u> .
(Appended System)	To read data from multiple databases, multiple System Definer activities must be created and linked serially. The successor System Definer activities defined is by default called Appended System.
Equilibrium Calculator	The Equilibrium Calculator activity is used to set thermodynamic conditions and to define axis variables when a series of equilibrium calculations are to be performed in one or more dimensions. Also see Equilibrium calculator.
Plot Renderer	The Plot Renderer activity is used to determine the layout of non-text based output. Also see <u>Plot renderer</u> .
Table Renderer	A table renderer activity is used for text based output. Also see <u>Table</u> renderer.
Binary Calculator	The Binary Calculator activity can be used for some calculations involving two components only. It can be thought of as a combination of a System Definer activity and an Equilibrium Calculator activity with certain adaptations to simplify the configuration of calculations on binary systems. Note that, to perform this activity successfully, you need a database that was designed for the Binary Calculator, such as the TCBIN database for example. Also see <u>Binary calculator</u> .
Ternary Calculator	The Ternary Calculator activity can be used for some calculations involving three components. It can be thought of as a combination of a System Definer activity and an Equilibrium Calculator activity with certain adaptations to simplify the configuration of calculations on ternary systems. Note that, to get a reliable result from performing this activity, you need a database that contains fully assessed binary and ternary systems. Also see <u>Ternary calculator</u> .



Activity type	Description
Scheil Calculator	The Scheil Calculator activity is used to perform Scheil-Gulliver calculations (also known as Scheil calculations). A default Scheil calculation is used to estimate the solidification range of an alloy assuming that i) the liquid phase is homogeneous at all times and ii) the diffusivity is zero in the solid. However, it is possible to disregard the second assumption for selected components. Also see <u>Scheil Calculator</u> .
Experimental File Reader	The Experimental File Reader activity can only be created from the top My Project node. This activity allows you to read an experimental data file (*.EXP). Such a file contains information specifying a plotted diagram, written in the DATAPLOT graphical language. See <u>Experimental file</u> <u>reader</u> .

2.2.3 Successor and predecessor nodes

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

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

Figure 3 is an example of a Project window where **Equilibrium Calculator 1** is the successor to **System Definer 1** and the predecessor to **Table Renderer 1** and **Equilibrium Calculator 2**.



Figure 3 An example of successors and predecessors.

2.3 Workflow

You can set up a whole *tree* in the **Project** window and then perform all the activities at once, or create and perform one activity at a time.

The typical workflow is the following:

• Define your system: Create a **System Definer** activity, which allows you to select a database and select which elements to have as components in your system. The database and elements are selected in the **Configuration** window.



- Set up and run your calculation: Create an **Equilibrium Calculator** activity, which allows you to set the conditions for your calculation (temperature, pressure, etc.) and set axis variables if you want to make a property or phase diagram. The settings of activities are specified in the **Configuration** window.
- Visualise the results: Create either a **Plot Renderer** or a **Table Renderer** activity that present the results of your calculation in diagram or table format. The results are shown in a **Plot Renderer** or a **Table Renderer** tab in the **Results** window. Note that if you do not visualise the results by performing a Plot Renderer or a Table Renderer, then you do not see any calculation results, even if you have performed an Equilibrium Calculator.

See <u>Working with Thermo-Calc projects</u> to get started.

2.4 The Graphical Mode buttons and menus

2.4.1 Main menu and toolbar

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

File Tools Window Help

□ □ □ □ □ ▲ Ď New Open Save Switch to Console Mode

Table 2 Main menu and toolbar options.

Option	Description	Action (s)
New	Create a new project.	Click New on the toolbar.
		Select File>New Project.
		Press Ctrl+N on the keyboard.
Open	Open an existing project.	Click Open on the toolbar.
		Select File>Open Project.
		Press Ctrl+O on the keyboard.
Save	Save a project. See <u>Saving and</u>	Click Save on the toolbar.
	opening Thermo-Calc project files.	Select File>Save Project.
		Press Ctrl+S on the keyboard.
Switch to	Open Console Mode.	Click the button to exit Graphical Mode and
Console Mode		open the Console Mode.
Append	Combine two projects into one	Select File>Append Project.
Project	project file.	
Save Project	Save an existing project with a	Select File>Save Project As
As	new name.	
Exit	Exit the program.	In the upper right-corner of the program, click the red X.
		Select File>Exit.
		Press Ctrl+Q on the keyboard.
Options	Change the global defaults for a	Select Tools>Options.
	variety of settings. See <u>Editing</u>	
	giobal defaults.	



Option	Description	Action (s)
Database Checker	Open the Database Checker, a program to check that the syntax of Thermo-Calc database files is correct. This is for advanced users who develop and manage databases.	Select Tools>Database Checker.
Window menu	Highlight a specific window on the GUI	From the Window menu, select an option to refocus on that specific window.
Show License Info	Open the License Information window. See <u>License</u> <u>information</u> and the <i>Thermo-</i> <i>Calc Installation Guide</i> for more information.	Select Help>Show License Info
Check for update	Check the Thermo-Calc Software website for updates to the software.	Select Help>Check for update

2.4.2 Project and activity menus

When working in the **Project** window you can right-click nodes to access menus with the available actions. For example, click the **My Project** node to open the menus shown in Figure 4. Most nodes in the tree have a common menu as shown in Figure 5, with differences based on the placement in the tree and the activity type.



Figure 4 Menu options available for the My Project node.

Create New Successor	System Definer
	Equilibrium Calculator Scheil Calculator
Perform Tree Now	
Perform Tree Later	
Rename	
Remove Clone Clone Tree	
Apply Auto Layout	
Snap to Grid	
Show Grid	
Zoom In	
Zoom Out	
Parat Zoom	

Figure 5 An example of the common menu for other activities.



Table 3 Menu options for activities.

Option	Description	Action (s)
Create New Activity	Add System Definer, Binary Calculator, Ternary Calculator, and Experimental File Reader nodes. See <u>Creating activities and successors</u> .	Right-click My Project and from the Create New Activity menu choose an option.
Create New Activity > Use Template	Choose from the available templates to use the Wizard or add predefined nodes. See <u>Using templates</u> .	Right-click My Project and from the Create New Activity>Use Templates menu choose an option. The templates are also available on the Configuration window, which you can access by clicking the My Project node, or from the Window menu.
Create New Successor	Add a successor to the selected node. Options are System Definer, Equilibrium Calculator or Scheil Calculator. See <u>Working with Thermo-Calc projects</u> and <u>Creating activities and successors</u> .	Right-click one of these nodes System Definer, Equilibrium Calculator, Binary Calculator, Ternary Calculator or Experimental File Reader, and from the Create New Successor menu choose an option.
Add a Predecessor	Add a predecessor to the selected node.	Right-click a node to add a predecessor to it (when available).
Perform Now or Perform Later	Perform a calculation or create a plot or table immediately, or schedule it for a time in the future. See <u>Performing</u> <u>projects, trees and activities</u> .	Right-click any node.
Rename	Change the name of the node.	Right-click any node.
Remove	Delete the selected node from the tree.	Right-click any node except My Project.
Clone	Duplicate the selected node and add it to the same tree. See <u>Cloning activities and</u> <u>trees</u> .	Right-click any node except My Project.
Clone tree	Duplicate a tree and add it to My project.	Right-click any node except My Project.
Apply Auto Layout	Apply an automatic layout to the nodes in the tree.	Right-click any node.
Snap to Grid	Snap a node to align it with the grid. See <u>Moving nodes in the tree and using the</u> grid.	Right-click any node.
Show Grid	Turn the grid on or off in the Project window.	Right-click any node.
Zoom In, Zoom Out, Reset Zoom	Zoom in and out of the Project window or reset the zoom to the default.	Right-click any node.

2.4.3 Moving windows

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

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



You can always go back to the standard window layout. From the main menu, select **Windows>Reset Windows**.

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

Button(s)	Description
Click to toggle on/off free-floating	
Image: Provide with the second sec	
_	Click to minimize an open window that has auto-hide turned on. Note that the window automatically minimizes if you select another window.
×	Click to close the window. You can open the window again from the Window main menu.

2.4.4 Moving nodes in the tree and using the grid

You can organise a project in the Project window in various ways.

- Selecting activities: Click an activity node to select it. To select several activities, hold down Ctrl while clicking on the activities you want to select. Alternatively, click and hold the mouse button while you trace a square around the activities that you want to select. Both the name and the icon that represents an activity must be within the square for it to get selected in this way.
- *Moving activities*: Click and hold the activity node, then move the cursor.
- *Zoom*: Use the scroll wheel to zoom in and out or in the **Project** window right-click and select **Zoom In** or **Zoom Out**. To go back to the default zoom, select **Reset Zoom**.
- *Turn on/off grid*: To show a grid of light-grey cross-hairs overlaid on a project (see Figure 6), click **Show Grid** in the toolbar. Click the button again to turn the grid off. Or right-click in the **Project** window and select **Show Grid**.
- Snap to grid: If you turn on Snap to Grid, each activity in the Project window is automatically positioned at a cross-hairs point in the grid. Click **Snap to Grid** in the toolbar or right-click in the **Project** window and select **Snap to Grid**.



Figure 6 The project window with the grid turned on and activity nodes moved from the default location.

2.4.5 Node status markers

Whether an activity is ready to be performed, is being performed, or has been performed is indicated by status markers overlaid on the activity icons in the Project window. The different status markers are shown on a System Definer icon.



Table 4 Node status markers for the Project and Scheduler windows.

Status marker	Location	Description
<u>kai</u>	Project window	No status marker means that the activity is ready to be performed and that it has not yet been performed.
· 📉	Scheduler window	No status marker means that the activity is scheduled to be performed but that Thermo-Calc has not yet begun to perform it.
1	Project window	A yellow triangle indicates that the activity cannot be run. The reason is that the necessary configurations for the activity have not been set or that other pre-requisites have not been met.
	Scheduler window	A yellow triangle indicates that there was an error during the performance of the activity.
1	Project window	A green disc indicates that the activity has been performed.
- <u>1</u>	Scheduler window	A green disc indicates that the activity has already been performed successfully.
·	Scheduler window	A green right-facing arrow indicates that the activity is being performed.
	Project window	A red circle with a dial (a clock face) indicates that the activity is currently being performed.

3. Working with Thermo-Calc projects

This section describes how you create and perform activities for your project, as well as how you manipulate and link various activities.

You work with Thermo-Calc in the Graphical Mode by creating, configuring and performing activities within a project. The activities in your project and how they are linked are represented as a tree-structure in the Project window, where you can also add new activities.

3.1 Using the Quick Start wizard

The **Quick Start** wizard gets you started using the Graphical Mode, even before you have any knowledge about how to work with Thermo-Calc projects. You can easily set up, calculate and visualise any of the following:

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

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

- 1. In the **Configuration** window click **Quick Start**. If you cannot see the **Quick Start** button, first click **My Project** in the **Project** window.
- 2. In the Select Project Type window click to select the type of calculation to perform. Single point equilibrium, Property diagram, Phase diagram or Scheil solidification simulation. Click Next.
- 3. In the **Define System** window, select a **Database** from the menu. TCFE7 is the default.
- 4. In the **Elements** section, click the check boxes of the elements to include as components in the system. Or click **Material file** to enter the file path to a material file or click the **Open** button to navigate to a file on the computer.
- 5. Click Next.



- 6. In the Select Conditions window, choose a Composition unit–Mass percent, Mole percent, Mass fraction or Mole fraction.
- 7. Under **Condition Definitions** specify the values of the state variables in the system.
- For a Property diagram or Phase diagram, specify the Axis Definitions of the stepping or mapping operation. Choose minimum and maximum values for the variable(s) (select Linear – min no. of steps, Linear – max step size or Logarithmic –scale factors) and whether it is Normal or Separate phases.
- 9. For a **Scheil solidification simulation**, and where applicable, select **Fast diffuser** to account for back-diffusion of any fast-diffusing elements.
- 10. Click Finish.
- 11. The Event Log window opens and shows information about the progress of the calculation.
- 12. The diagram is plotted in a **Plot Renderer** tab in the **Results** window. If you have calculated a single-point equilibrium, then a **Table Renderer** tab shows information about the equilibrium.
- 13. To save the project, click **Save** on the main toolbar. To save a diagram or table, rightclick the diagram or table and select **Save As**.

3.2 Using templates

Use a Template to create all the activities necessary for a certain type of calculation. In the **Project** window click the **My Project** node to display the templates in the **Configuration** window as in Figure 7.



Figure 7 The templates available in the Configuration window.

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

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



You can also select templates from the Project window by right-clicking the topmost **My Project** node, choosing **Create New Activity**, and opening the **Use Template** submenu.

3.3 Saving and opening Thermo-Calc project files

Thermo-Calc makes use of project files with the file name suffix .TCU. To save your project and all its settings and results, on the toolbar click **Save**. Select to **Include calculated results in the project file** (the default) or not. To open a Thermo-Calc project file, on the toolbar click **Open** and select the project file in the **Open file** window.

You can only have one project file open at a time. However, you can attach the trees from additional project files to the topmost My Project node. To append an additional project file in this way, from the main menu select File>**Append Project** and open a project file.

3.4 Creating activities and successors

You can create a new activity in the following ways:

In the Project window, right-click an activity and choose Create New Activity (My Project node only) or Create New Successor (all other nodes). Select the activity you want to create from the submenu.
 At the bottom of the Configuration window, click Create New Activity or Create New Successor and select the activity to create.

3.4.1 Cloning activities and trees

You can clone a single selected activity or the selected activity and all the activities that succeed it. The predecessor of the selected activity also is the predecessor of the clone. Cloned activities are configured exactly like the activities that they were cloned from, and any results of calculations or plots are also cloned. To clone a selected activity, right-click the activity and select **Clone**.

For example, if you clone the Equilibrium Calculator in this project:



Figure 8 Cloning an Equilibrium Calculator activity node.

The result is that **Equilibrium Calculator 2** is created as a successor to **System Definer 1**. The new Equilibrium Calculator has exactly the same settings for conditions, functions and options as Equilibrium Calculator 1 from which it was cloned. If the Equilibrium Calculator is done already, then the calculation results are also cloned. If the activity is a Plot Renderer or a Table Renderer, then the plot or table is cloned. If you also want to clone all the successor activities that follow a selected activity, then right-click and select **Clone Tree** instead. See <u>Equilibrium Calculator clones and successors</u> for more information.





3.4.2 Equilibrium Calculator clones and successors

If you create an Equilibrium Calculator as a successor to another Equilibrium Calculator, then the successor inherits all the settings for conditions, functions and options from its predecessor. In this respect, it is similar to a clone. However, the successor is different from a clone in that it *does not inherit any calculated results and it is a successor to the Equilibrium Calculator instead of a successor to its predecessor*. The calculated result from an Equilibrium Calculator that is the predecessor to another Equilibrium Calculator is the starting value for the latter's calculation. The clone of an Equilibrium Calculator on the other hand, does not receive any data as input from the Equilibrium Calculator that it was cloned from.

For an example of how serially coupled Equilibrium Calculators can be used, see example 6 in the *Thermo-Calc Graphical Examples Collection*.

3.5 Performing projects, trees and activities

You can trigger the performance of an activity and all the activities below it in the same tree in either the Project window or in the Configuration window. In the Project window you can also perform a single activity without performing its successors or perform the whole project (all the activity trees).

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

Whenever you perform an activity, all activities that must be performed as a prerequisite to the performance of that activity are automatically performed first. Consequently, if you perform a Plot Renderer with an Equilibrium Calculator and a System Definer above it in the activity tree, then the System Definer and the Equilibrium Calculator are automatically performed first.

In the **Project** window, you can do any of the following:

• *Perform an activity*: Right-click the activity and select **Perform Now**, or **Perform Later** and schedule a time when the activity is performed.

🔺 Select time	X
Perform in:	
þ hours 30 → minutes	
OK Cancel	

- *Perform an activity and all activities below it in the tree*: Right-click any activity in the tree that you want to perform and select **Perform Tree Now**. Or select **Perform Tree Later** and schedule a time when all the activities in the tree are performed.
- *Perform a project*: Right-click the **My Project** node and select **Perform Now** or **Perform Later** and schedule a time for all the activity trees in your project to be performed.



If there is an error during the performance of an activity, icons display status markers, which are described in <u>Node status markers</u>.

3.5.1 Using the Scheduler

The Scheduler window shows information about activities that Thermo-Calc is currently performing or are scheduled to be done. It also indicates if there is an error during performance and an activity is aborted. If you have set an activity, tree or project to be performed at a later time (with the **Perform Later** or **Perform Tree Later** options) then this scheduled performance is listed as well.

Whenever you trigger the performance of a whole project, tree or individual activity, all the activities to be performed are presented under a Job heading. If all the activities belonging to a job are successfully completed the job and its activities disappear from the Scheduler window.

If there is an error during the performance of an activity, icons for that job and activity remain in the Scheduler window until removed. See <u>Node status markers</u> for these indicators.

Scheduler	L	X
🔅 Scheduled Jobs		
🚊 🕕 🕕 Job no 1		
Equilibrium Calculator 3 (127.0.0.1)		
🚊 🧈 Job no 2		
. Stable and metastable FE-C phase diagram		
Equilibrium Calculator 2		
Equilibrium Calculator 1 (127.0.0.1)		

Figure 9 An example of a list of scheduled jobs.

3.5.2 Managing the schedule

In the Scheduler window, you can cancel scheduled jobs, remove errors and show information about errors.

- *Cancel All Jobs*: To cancel all jobs, right-click the **Scheduled Jobs** label or the cogwheel icon, and select **Cancel All Jobs**.
- *Clear All Errors*: To remove all failed activities and jobs, right-click the **Scheduled Jobs** label or the cogwheel icon, and select **Clear All Errors**.
- *Cancel Job*: To cancel a specific job, right-click the job label (for example, **Job no 1**) and select **Cancel Job**.
- *Clear Error*: To remove a specific failed job, right-click the job label (for example, Job no 1) and select Cancel Job.
- *Show Error Log*: To open a window with information about an error, right-click the label for the failed job (for example, **Job no 1**), and select **Show Error Log**.

3.5.3 The Event Log

The **Event Log** window is closed by default, but is opened when an activity, tree or project is performed.

Information about what Thermo-Calc is currently doing is shown in blue, and error and warning messages are shown in red.

You can specify how detailed the information in the Event Log window by opening the **Options** window, and from the main menu selecting **Tools>Options>General** tab and setting the **Log level** slide bar to anything between **Debug** (most detailed) and **Error** (least detailed).



Event Log	×
14:50:34,751 INFO Cancelling activity: Equilibrium Calculator 1	~
14:50:34,751 INFO Cancelling activity: Plot Renderer 1	
14:50:36,266 WARN The subprocess completed with status code 2: the execution was	3
cancelled by the user	
14:50:36,376 ERROR Gobbled: 14:50:36,376 ERROR Error when executing the activity	
Error when sending a remote event: Software caused connection abort: socket w	
rite error	
14:50:36,594 WARN The subprocess completed with status code 2: the exec	
ution was cancelled by the user	
15:36:25,495 INFO Activity was renamed to Appended System 1	\checkmark

Figure 10 An example of an Event Log.

4. Activities

In this section is a description of each type of activity, brief descriptions of the Configuration window settings, and descriptions of some procedures that are tied to specific activities.

4.1 System definer

In a System Definer activity, you select which database to use for retrieving thermodynamic data, and define which elements your system has as components. You can also select which species to include as well as change the reference temperature and pressure for your components.

4.1.1 Predecessors and successors

- Possible predecessors: My Project System Definer
- Possible successors: System Definer, Equilibrium Calculator, Scheil Calculator

A System Definer that is a successor to another System Definer by default gets the name **Appended System**.

4.1.2 Selecting a database and defining elements

This procedure describes how to define a system, namely select a database and defining the elements that are in the system. You must have created and selected a System Definer activity in the Project window.

1. In the **Configuration** window, from the top menu, select the database to use from the **Select database** menu.



									S 🚽	ysten	n Def	iner 1	L					
t dat	abase:	TCFE	7			v		Open u	iser da	tabase	2							
ote	Carada	Dh		ad phy						Data (_				
165	Specie	es Ph	ases a	ind Pha	ase Co	nstitut	ion C	.ompor	ients	Data :	source	s De	scriptio	n				
					Period	ic Table	e	Alph	abetic	List	M	lateria						
											1							
									ZE	VA								
н										/-							He	
Li	Be											в	С	Ν	0	F	Ne	
Na	Mg											AI	Si	Р	S	CI	Ar	
к	Са	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
RЬ	Sr	Y	Zr	Nb	Мо	То	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I.	Xe	
Cs	Ва	*	Hf	Та	w	Re	Os	Ir	Pt	Au	Hg	ті	Pb	Bi	Po	At	Rn	
Fr	Ra	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	FI	Uup	Lv	Uus	Uuo	
Lant	thanide	series	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	ТЬ	Dy	Но	Er	Tm	Yb	Lu	
Ad	ctinide s	eries	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	
		Г		10	_		_											

- 2. In the **Elements** tab, click the elements in the periodic table (or on the alphabetic list) that you want to include in your system.
- 3. If required, you can change species, phases or components in the other tabs.
- 4. Click **Perform** to start the System Definer activity immediately and retrieve thermodynamic data about your system.

4.1.3 Appending data from an additional database

If you want to use thermodynamic data from several databases, you can create extra System Definers as successors to your first System Definer. You must already have created a System Definer.

- 1. In the **Project** window, right-click the System Definer to which you want to append thermodynamic data. Choose **Create New Successor>System Definer**.
- 2. Or select the System Definer in the **Project** window, and at the bottom of the **Configuration** window click **Create New Successor> System Definer**. This creates an Appended System activity, which is linked to a System Definer predecessor.
- 3. In the **Configuration** window for the Appended System, select which database you want to append thermodynamic data from, regarding which components, phases, etc.

4.2 Equilibrium Calculator

An Equilibrium Calculator allows you to set the conditions for, and perform, a calculation. The **Configuration** window for an Equilibrium Calculator has these tabs:

- **Conditions**: Set the conditions for your calculation that define the stepping or mapping axis variables. This tab can be viewed in a simplified mode and in an advanced mode.
- **Functions**: Define your own quantities and functions, which you then can calculate and plot.
- **Options**: Modify numerical settings that determine how equilibria are calculated, as well as how stepping and mapping calculations are performed.



4.2.1 Predecessors and successors

Possible predecessors: System Definer, Equilibrium Calculator

Possible successors: Plot Renderer, Table Renderer, Equilibrium Calculator

An Equilibrium Calculator that is the successor of another Equilibrium Calculator inherits all the Configuration window settings of the predecessor.

For an example of how serially coupled Equilibrium Calculators can be used, see example 6 in the *Thermo-Calc Graphical Examples Collection*.

4.2.2 Setting conditions for different calculations

Conditions and axis variables are set in the Conditions tab of the Configuration window. There you can specify the conditions and axis variables you want to use for your calculation. The tab can be viewed in two modes, the simplified mode (default) or the advanced mode.

What conditions you have to set depends on the type of calculation you intend to perform.

For examples of how various kinds of calculations can be set up using an Equilibrium Calculator, see the *Thermo-Calc Graphical Examples Collection*: example 1 is an example of a single-point equilibrium calculation; example 2 an example of a stepping calculation; and example 5 is an example of a mapping calculation.

Configuration						
		🔳 Equil	ibrium Calcu	lator 1		
Conditions Function	ons Options					
Composition unit	lass percent	▼]		Switch to advanced mode		
Condition Definition	ons					
Temperature	Kel	vin 👻	1000.0			
Pressure	Pas	scal 👻	100000.0			
System size	Mo	le 🔹	1.0			
Composition	Fe		99.98			
Composition	С		0.01			
Composition	Cr		0.01			
Calculation Type Single equilibrium Property diagram Property grid Phase diagram 						
Axis Definitions Quantity	Min	Max	Step division	Туре		
Temperature 👻	500.0	3000.0	50	Linear - min no. of steps 👻		
Mass perc 👻	0.0	100.0	50	Linear - min no. of steps 👻		
		Add Predeces	sor Perfo	rm Create New Successor >		
				•		

The following table briefly describes what you can set on the Conditions tab in simplified mode. More advanced options are available if you click **Switch to advanced mode**.



Setting or condition	Description
Composition unit	Select whether to use mass percent, mole percent, mass fraction or mole fraction when defining the composition of your system.
Condition definitions	Specify the values (and units) of the different state variables.
Temperature	
Pressure	
System size	
Composition	
Calculation type	Select whether to calculate a single equilibrium (no axes), a
Single equilibrium	property diagram, a property grid or a phase diagram.
Property diagram	
Property grid	
Phase diagram	
Axis definitions	To calculate a property diagram, a property grid or a phase
(X-axis)	diagram, define the axis variable (property diagram) or the two
(Y-axis)	axis variables (property grid and phase diagram).
	the stepping/mapping to apply to and set the minimum and maximum values.
	Note that if the Equilibrium Calculator already has a Plot Renderer as a successor and you change the stepping/mapping quantities, then the quantities represented on the X- and Y-axis is automatically updated in the Plot Renderer.
Step Division and Type (Property diagram/Phase diagram)	If you set Type to Linear - min no. of steps , then the Step Division value specifies at minimum number of steps that is calculated between the minimum and maximum value during the stepping/mapping operation.
	If you set Type to Linear - max step size , then the Step Division sets the maximum size of each step.
	If you set Type to Logarithmic - scale factor , then Step Division specifies the scale factor of a logarithmic function that distributes the steps from the initial equilibrium to the minimum and maximum values you have defines.
Normal / Separate phases / T- Zero	To do the stepping operation along an axis one phase at a time, select Separate phases .
	If you want to calculate the T_0 -line, where the Gibbs energy for each phase is the same, then select T-Zero .
Number of steps (Property grid)	When calculating a property grid, you set a fixed Number of steps instead of a Step Division value and Type for each axis. The number of steps along with the minimum and maximum values for the axes define a grid. For each grid point, Thermo- Calc calculates an equilibrium.



4.2.3 Setting conditions – advanced mode

In advanced mode, you can add and remove conditions as you see fit. Furthermore, you can define additional axis definitions beyond the two that you can set in simplified mode. However, the number and types of conditions that you set must still conform to the Gibbs' phase rule (see *Thermo-Calc Educational Material*). The **Number of missing conditions is** field, at the top of the tab shows how many conditions that you have left to set. If the number is negative, then you need to remove that number of conditions.

The next section demonstrates how to calculate and plot a diagram with a fixed phase in order to find out, for example, at what temperature a material starts to melt.

4.2.4 How to calculate with a fixed phase

This section describes how you use the advanced mode to set a certain phase to be fixed at a certain amount. This allows you to, for example, find out at what temperature you material starts to melt. If you set the phase to be fixed to liquid phase at zero amount, and leave the temperature state variable undefined, then you can calculate at what temperature the material enters a state where the liquid phase is no longer zero (that is when it starts to melt).

When you perform an equilibrium calculation with a fixed phase, it is recommended to do it in an Equilibrium Calculator that is the successor to an Equilibrium Calculator that performs an ordinary equilibrium calculation for which you roughly estimate the value of the condition you are interested in. This provides your fixed phase calculation with better starting values.

- 1. Create an Equilibrium Calculator and have this activity selected in the Project window.
- 2. In the **Configuration** window, click **Switch to advanced mode**. Note, if you have set **Default calculation mode** to **Advanced** in the Calculation tab of the Options window, then the **Configuration** window is in advanced mode by default, see section 2.4.4.
- 3. Click the green + button to add a condition.
- 4. Select **Fix phase** from the first menu.
- 5. Select the phase that you want to fix in the second menu, and set the amount of that phase you want to fix the phase to. For example, if you want to know when your material starts to melt, set the phase to **LIQUID** and the value to **0.0**, as shown below:

lumber of missing conditions is -1		Switch to simplified mode	
Condition Definitions Image: Operature	*	Kelvin y 1000.0	^
🖸 🤤 🗹 Fix phase	~		

- 6. Above the condition definitions, the Number of missing conditions is field is probably 1. This means that you must remove one condition.
- 7. To remove a condition, either click the red (-) button, or unselect it by clicking in the tick-box. For example, if you want to know at what temperature your material starts to melt, then you cannot have a fixed temperature. For example, the temperature condition is not selected:

Conditions Functions Options		
Number of missing conditions is 0		Switch to simplified mode
Condition Definitions		^
😳 😑 🔲 Temperature	✓ Kelvin ✓ 1000.0	
😳 🤤 🗹 Fix phase	✓ LIQUID ✓ 0.0	

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



4.2.5 Calculating and plotting functions

The Functions tab allows you to define your own functions that you can then set to be plotted in a Plot Renderer.

For an example of how you can use functions that you yourself define, see example 7 in the *Thermo-Calc Graphical Examples Collection*.

You must have created an Equilibrium Calculator and you must have this activity selected in the Project window.

- 1 Create an Equilibrium Calculator and have this activity selected in the Project window.
- 2 In the **Configuration** window, click the **Functions** tab.
- 3 Under **Quantity Definitions**, define any number of quantities. These quantities are referred to as **Q1**, **Q2**, **Q3** and so on. When you have defined a quantity, you can use it to define functions under **Function definitions**.

Configuration	
Equilibrium Calculator 1	
Conditions Ellipctions Options	
Quantity Definitions	
© Q1 = Amount of phase	~
Function Definitions	
S S Traction_solid = 1-Q1	
Add Predecessor Perform Create New Successor >	

In this screen shot, the quantity Q1 is defined as the amount of liquid phase. This quantity is then used to define a function called **fraction_solid**, which gives as its output the fraction of solid phase (that is 1-Q1).

- 4 Under **Function Definitions**, define as many functions as you need. Enter the name of each function in the left field before the equal sign (=), and enter the function itself in the right field after the equal sign. Note that you can also use Console Mode syntax when entering the function. For example, the function above could have been entered as **1-NP(LIQUID)**.
- 5 To set up a Plot Renderer so that it plots the defined function, create a Plot Renderer as a successor to the Equilibrium Calculator in which you have defined the function.



6 In the tab for the Equilibrium Calculator that contain the function, set one of the axis variables to **Function**, then select the name of the function you have defined from the menu. In the example below, the Y-axis is set to plot the value of the function **fraction_solid**.

Configuration	
🖄 Plot Renderer 1	
Save Diagram Show Triangular Show Grid Switch Axes	
Kequilibrium Calculator 1	
Tie lines: 0 🗢 Legend option: Axis quantity 🗸	
X Axis	
Axis variable: Temperature v Kelvin v	
Axis type: Linear 🗸	
Limits: 1500.0 to 1700.0	
YAxis	
Axis variable: Function v fraction_solid v 1-Q1	
Axis type: Linear 🗸	
Limits: 0.0 to 1.0 Automatic scaling	
Add Predecessor Perform Create New Successor	>
<	>

7 When run, the Plot Renderer plots the value of the function.

4.3 Plot renderer

The Plot Renderer allows you to set the plotting axis variables for property and phase diagrams. If you are plotting a property grid, then the X- and Y-axes always represent the quantities that define the stepping axes in the Equilibrium Calculator, but you need to set a variable for the Z-axis (the axis perpendicular to the plane defined by the X- and Y-axes).

Several Plot Renderer activities (as well as Table Renderer activities) can be shown in the Results window as different tabs, as the following screen shot shows:





If you have plotted a diagram and then modify something in the tree that the Plot Renderer is associated with, then a notification sign—an exclamation mark enclosed in a yellow triangle—is shown in the Plot Renderer's tab. The following screenshot shows a property grid diagram that has not been updated in light of changes made to the activity tree that the Plot Renderer belongs to.



4.3.1 Predecessors and successors

Possible predecessors Equilibrium Calculator Binary Calculator Ternary Calculator Scheil Calculator Experimental File Reader

Possible successors None

The configurations that can be set in the Configuration window for a Plot Renderer vary depending on the kind of predecessor it is created from.

A Plot Renderer can have several predecessors (if you want to plot several calculations in the same diagram), in which case there are several tabs in the Configuration window, one for each predecessor.



4.3.2 Configuration window settings

The following screenshot shows the **Configuration** window for a Plot Renderer that is the successor to an Equilibrium Calculator.

Configuration		
	🖄 Plot Renderer 1	
Save Diagram	Show Triangular Show Grid Switch Axes Retain Labels	
🖄 Equilibrium	Calculator 1	
Tie lines:	1 → Legend option: Stable phases ▼	
X Axis		
Axis variable:	Composition Fe Mass percent	
Axis type:	Linear 🔻	
Limits:	0.0 to 100.0 step 10.0 📝 Automatic scaling	
Y Axis		
Axis variable:	Temperature Kelvin	
Axis type:	Linear 🔻	
Limits:	500.0 to 3000.0 step 250.0 📝 Automatic scaling	
	Add Predecessor Perform Create New Successor >	

The following table briefly describes the configurations that can be set in the Configuration window.

Setting/Button	Description
Save Diagram	Save the plot diagram.
Show Triangular	Display the diagram in triangular form, with the X-axis along the base and the Y-axis along the left side. Such a diagram is often useful if you want to plot the fractions of two components in a ternary diagram.
Show Grid	Overlay a grid on the diagram.
Switch Axes	Show the plotting X axis variable on the diagram's Y-axis, and the Y axis variable on the diagram's X-axis.
Retain Labels	Toggle the default to keep labels displaying on the plot. By default labels are retained.
Tie lines	Select how many tie lines to be plotted in the diagram. Every <i>n</i> th number of tie line is plotted, where <i>n</i> is the number set here. Consequently, the higher the number, the fewer the number of plotted tie lines in the diagram.
	Note that this setting is not present if the Plot Renderer is a successor to a Scheil Calculator or to an Equilibrium Calculator where only one axis has been defined and varied (that is, an Equilibrium Calculator that has performed a stepping calculation).
Legend option	Select whether the diagram's legend should display the Stable phases or the Axis quantity .



Setting/Button	Description					
Plot type	This menu is only available if the Plot Renderer is a successor to an Equilibrium Calculator that has been set up to calculate a property grid. Choose either Heat map or Contour .					
	On a heat map diagram, each equilibrium calculation in the grid is represented by a colour-coded pixel, where dark red represents the highest Z-axis variable value and dark blue represents the lowest Z-axis variable value.					
	On a contour diagram, Z-axis variable values are traced with curves in different colours (in the same way that height values are traced with curves on a topographical map).					
Axis variable	Set which state variable that you want plotted along the X-axis and the Y-axis.					
	Note that if the stepping/mapping variables are changed in the Equilibrium Calculator that precedes the Plot Renderer, then the variables to be plotted along the diagram's X- and Y-axis are automatically updated to the appropriate quantities.					
Axis type	Select what type of scale to use on the axis. Choose between Linear, Logarithmic, Logarithmic 10 and Inverse.					
Limits	Specify the range along the axis that should be shown in the plot by setting the minimum and maximum values of the axis variable. You can also determine the step size between the tick marks along each axis. Alternatively, select Automatic scaling .					

4.3.3 Adding labels

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

You can enter the label as **Plain text** or **LaTeX-formatted text**. For **Plain text**, and when applicable, choose an option from the list.

For **LaTeX-formatted text** the chosen point name is added by default. Use the LaTeX math text to enter or edit the text as required. For example, underscores (_) are added before the 2 and 4 to make subscripts in the label.



For a list of supported LaTeX commands, see:

http://www2.ph.ed.ac.uk/snuggletex/documentation/mathmode.htmlhttp://www.thermocalc.com/products-services/software/systemrequirements/.

🔺 Edit Labe	el	×
Laboli		
Label.	CA_2SIO_4 ALPHA+HATRURITE	LaTex-formatted text 🔻
Text size:	16 -	
Rotation and	gle: 0.0	
	Show anchor	
	Show details	
	OK Cancel Reset Delete	



In this example, you must also remove the underscore after the 4 in order to make it work correctly on the plot.

The suggested label specifies the names of the stable phases at the coordinate where you clicked. Once a label is created, you can select it and move it around on top of the diagram. By default the **Show anchor** check box is selected: there is always an arrow from the label point to the coordinates.

If you do not want the label to be oriented horizontally in the Plot Renderer tab, then you specify the number of degrees that it should be rotated in the **Rotation angle** field.

4.3.4 Changing the plot properties



For global changes to the default settings plots see <u>Plotting: Change</u> <u>the default settings for any plotted diagrams</u>. The settings are the same but applied to all new plots.

To make local changes to the appearance of a specific plot, in the **Results** window right-click a plot and select **Properties**. In the **Plot Properties** window the settings in the table below can be made.

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

4.3.5 Saving your diagram

To save a diagram, at the top of the **Configuration** window click **Save Diagram**. Or right-click the diagram in the **Results** window and select **Save As**.

4.3.6 Plotting several calculations in one diagram

It is possible to plot several calculations in one and same diagram by adding extra predecessors to the Plot Renderer activity.

For an example of a project in which several calculations are plotted in one diagram, see example 5 in the *Thermo-Calc Graphical Examples Collection*.

To plot several calculations in one diagram, you must have, in addition to the Plot Renderer's original predecessor, at least one extra possible Plot Renderer predecessor in your project. The extra predecessor can be an Equilibrium Calculator, a Binary Calculator, a Ternary Calculator, a Scheil Calculator or an Experimental File Reader.



 Select the Plot Renderer activity in the Project window, and click Add Predecessor in the Configuration window. Or right-click the Plot Renderer and choose Add Predecessor then select which predecessor to add.

My Project	System Definer.	2
System Definer 1	* .	
	Equilibrium Calculator 2	
Equilibrium Calcul	lator 1	Scheil Calculator 1
	-	
Plot Rendere	Add Predecessor	Equilibrium Calculator 2
	Perform Now	Scheil Calculator 1

2 When selected, the extra predecessor becomes linked to the Plot Renderer in the Project window. On the Plot Renderer's Configuration window, the different predecessors are shown as two different tabs:

		##	1					
Save Diagram	Show Triangul	ar Show Grid Sv	witch Axes					
Equilibrium Calculator 2 🖄 Equilibrium Calculator 3								
Tie lines:	1 🗢	Legend option:	Axis quant	ity 🗸				
XAxis								

- 3 Configure how you want each calculation plotted on the tabs in the **Configuration** window, then perform the Plot Renderer activity.
- 4 The calculations are plotted in the same diagram in a tab in the **Results** window. If any of the axis variables of the plots differ, then the label and scale of all calculations are shown parallel to each other. The following screen shot shows a diagram in which two calculations with different plotting axes variables have been plotted.





4.4 Table renderer

A Table Renderer visualises the result of calculation as a table. Several Table Renderer activities (as well as Plot Renderer activities) can be shown in the Results window as different tabs.

You can only successfully tabulate the results of a single-equilibrium calculation or a stepping operation. The tabulated data from an equilibrium calculation is very different from the tabulated data from a stepping calculation.

4.4.1 Predecessors and successors

Possible predecessors Equilibrium Calculator

Possible successors None

4.4.2 Tabulated results from an equilibrium calculation

The following tab shows the result of an equilibrium calculation.



Results				٦	l ×
Table Renderer 1	Table Rendere	r 2			
System					
Moles	1.00000	_			
Mass	55.82663	[Gram]			
Temperature	1000.00000	[Kelvin]			
Total Gibbs Energy	-42264.29819	[Joules]			
Enthalpy	24732.95322	[Joules]			
Volume	7.31246E-6	[Cubic meter]			
Component	Mole Fraction	Mass Fraction	Activity	Potential	
Fe	0.99954	0.99990	0.00619	-42276.35352	
С	0.00046	0.00010	0.14013	-16339.51682	
Stable Phases					
	Moles	Mass	Volume Fraction		
BCC_A2#1	1.00000	55.82663	1.00000	Composition and constitution	~
Composition					
Component	Mole Fraction	Mass Fraction			
Fe	0.99954	0.99990			
с	0.00046	0.00010			
Constitution	(Fe), (C, VA),				
	Constituent	Site Fraction			
Sublattice 1:					
	Fe	1.00000			
Sublattice 2:					
	VA	0.99984			
	c	0.00016			
	-	0.00010			

For each stable phase that is listed, you can select in the menu displaying **Composition and constitution** in the screen shot how much information you want to view. In the preceding screen shot, the maximum amount of information is shown, that is, information about both composition and constitution.

4.4.3 Tabulated results from a stepping operation

The following tab shows the results of a stepping calculation.



Results			E	. ×
Table Renderer 1	Table Renderer 2			
Temperature [Kelvin]	Amount of LIQUID [Mole]	Amount of FCC_A1 [Mole]	Amount of BCC_A2 [Mole]	A
1670.00000		1.00000		
1675.05758		1.00000		
1675.05758		1.00000	0.00000E0	
1680.00000		0.30541	0.69459	
1684.78866		0.00000E0	1.00000	
1684.78866			1.00000	
1690.00000			1.00000	
1700.00000			1.00000	
1710.00000			1.00000	
1720.00000			1.00000	
1730.00000			1.00000	
1740.00000			1.00000	
1750.00000			1.00000	
1760.00000			1.00000	
1770.00000			1.00000	
1780.00000			1.00000	
1790.00000			1.00000	
1800.00000			1.00000	
1806.61591			1.00000	
1806.61591	0.00000E0		1.00000	
1810.00000	0.75046		0.24954	
1810.19674	1.00000		0.00000E0	
1810.19674	1.00000			×
<	•			>

Defining columns

In the **Configuration** window set the columns you want the table to contain:

		Table Renderer 1											
Save table	Decimal digits: 5 🗢	Number format: Auto 🗸											
Columns	emperature	V Kelvin V											
00	Amount of phase	V No normalization V All phases V Mole	~										

4.4.4 Setting number format and number of decimal digits

The results can be presented in ordinary decimal number format or using normalized scientific notion. Set this in the **Number format** menu in the **Configuration** window. You can also select **Auto** and Thermo-Calc uses the most appropriate format given by the tabulated data.

You can also increase or decrease the number of decimal digits that are used in the table: this is in the **Decimal digits** field in the **Configuration** window.

4.4.5 Setting background colours

By right-clicking a Table Renderer tab in the **Results** window, and selecting **Properties** from the pop-up menu, you can change the background colours of the table.

4.4.6 Saving tabulated data

To save all the data in a table as a plain text file, click **Save table** in the **Configuration** window or right-click in the table in the **Results** window and select **Save As**.

To copy the data from a single cell of a table to the clipboard, right-click the cell and select **Copy**. To copy the whole table to the clipboard, select **Copy all**.

Saved data is the data shown in the **Table Renderer** tab. If you have calculated data but not displayed it, this is not saved.



4.5 Experimental file reader

The Experimental File Reader activity can only be created from the top My Project node. This activity allows you to read an experimental data file (*.EXP). Such a file contains information specifying a plotted diagram, written in the DATAPLOT graphical language.

4.5.1 Predecessors and successors

Possible predecessors My project

Possible successors Plot Renderer

4.5.2 Plotting an experimental data file

- 1. Right-click **My Project** and from the **Create New Activity** submenu choose **Experimental File Reader**.
- 2. In the **Configuration** window in the **EXP file** field, enter the name of EXP-file that you want to plot.
- 3. Click **Create New Successor** and select **Plot Renderer**. Or right-click the experimental file reader activity in the Project window and from the **Create New Successor** submenu choose **Plot Renderer**.
- 4. Click **Perform** in the **Configuration** window or right-click the plot renderer activity that you created in the **Project** window.

4.6 Binary calculator

A Binary Calculator can be used for some calculations involving two components. You can think of this activity as a combination of a System Definer and an Equilibrium Calculator, but designed to simplify setting up and performing calculations on binary systems.

The Binary Calculator relies on some specifications that are not supported by all databases. You therefore need a database that was designed for the Binary Calculator, such as the TCBIN database for example.

For an example of how a Binary Calculator can be used in a project, see example 3 in the *Thermo-Calc Graphical Examples Collection*.

4.6.1 Predecessors and successors

Possible predecessors My Project

Possible successors Plot Renderer

4.6.2 Configuration window settings

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



Configur	Configuration																
	🔁 Binary Calculator 1																
Select d	Select database: TCBIN V Open user database																
Element	Elements Phases and Phase Constitution Data Sources Description																
	75 14																
н										-							He
Li	Be											В	С	Ν	0	F	Ne
Na	Mg											AI	Si	Ρ	s	CI	Ar
к	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Мо	Тс	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	Т	Xe
Cs	Ва	*	Hf	Та	w	Re	Os	Ir	Pt	Au	Hg	ті	Pb	Bi	Po	At	Rn
Fr	Ra	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	FI	Uup	Lv	Uus	Uuo
• Lan	thanide	series	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dv	Но	Er	Tm	Yb	Lu
Ad	tinide s	eries	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr
Calcula	tion Ty	/pe															
O Phas	e diag	ram															
Gibb	s ener	gy curv	ves	Tempe	rature	Kelvir	ı	~ 1	000.0								
Activ	ity cu	rves		Tempe	rature	Kelvir	1	v 1	000.0								
O Phas	e frac	tions		Mole fr	action	Та		v 0	.0								
			<u> </u>	Au	urreu	ecesso		Calcu	arte Al	avity	carve	, L	creat	CINEW	Jucce	3301	

The following table briefly describes the available settings that must be configured before performing the calculation.

Setting	Description
Select database	Select a database that contains specifications dedicated to the Binary Calculator.
Elements	In the periodic table, select the two elements that make up the
(periodic table)	components of the system.
Phase diagram	Select to perform a mapping calculation.
Gibbs energy curves	Select the temperature; the Gibbs energy curves are calculated at a constant temperature over the whole composition range.
Activity curves	Select the temperature; the activity curves are calculated at a constant temperature over the whole composition range.
Phase fractions	Select the composition; the phase fractions are calculated as a function of temperature at a constant composition.

4.7 Ternary calculator

A Ternary Calculator can be used for some calculations involving three components. You can think of this activity as a combination of a System Definer and an Equilibrium Calculator, but designed to simplify setting up and performing calculations on ternary systems.



For an example of how a Ternary Calculator can be used in a project, see example 4 in the *Thermo-Calc Graphical Examples Collection*.

4.7.1 Predecessors and successors

Possible predecessors My Project

Possible successors Plot Renderer

4.7.2 Configuration window settings

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

Configur	onfiguration										L ×						
	Ternary Calculator 1																
Select d	Select database: TCFE7 v Open user database																
Element	lements Phases and Phase Constitution Data Sources Description																
Н										-							He
Li	Be											В	С	Ν	0	F	Ne
Na	Mg											AI	Si	Р	S	CI	Ar
К	Са	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Мо	Тс	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I.	Xe
Cs	Ba	*	Hf	Та	W	Re	Os	Ir	Pt	Au	Hg	ті	Pb	Bi	Po	At	Rn
Fr	Ra	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	FI	Uup	Lv	Uus	Uuo
• Lan	thanide	series	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	ть	Dy	Но	Er	Tm	Yb	Lu
Ad	ctinide s	eries	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr
Calcula Isoti Mon Liqui	alculation Type) Isothermal section Temperature Kelvin Monovariant lines) Liquidus projection Temperature Kelvin Vin 298.15 Max 3273.15 Interval 100.0																
	0			<	A	Add Pre	deces	sor	Per	form	C	reate I	New Si	uccesso	or	>	

The following table briefly describes the available settings that must be configured before you perform the calculation.

Setting	Description
Select database	Select a database that contains specifications dedicated to the Ternary Calculator.
Elements	In the periodic table, select the three elements that make up
(periodic table)	the components of the system.
Isothermal section	Select the temperature at which the ternary system is
	calculated for the whole composition range.
Monovariant lines	The variation of the liquid compositions with temperature is calculated.
Liquidus projection	Select the desired temperature range and a temperature
	interval. The projection liquid surface and the monovariant lines are calculated over the given temperature range.



4.8 Scheil Calculator

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

For an example of how a Scheil Calculator can be used in a project, see example 8 in the *Thermo-Calc Graphical Examples Collection*.

4.8.1 Predecessors and successors

Possible predecessors System Definer

Possible successors Plot Renderer

By default, a Plot Renderer successor has the default plot axes **Mole fraction of solid** (X-axis) and **Temperature Celsius** (Y-axis). When these default axes are used in the Plot Renderer, the results of normal equilibria calculations are automatically plotted in the same diagram as the Scheil calculations.

4.8.2 Configuration window settings

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

Configuration		
		Scheil Calculator 1
Start temperature 2	2500.0 Temperature step 1	.0 Temperature unit Kelvin v
Allow BCC \rightarrow FCC	Composition unit Mass percent	v
Composition Fe	99.99 Fast diffuser	
Composition C	0.01 Fast diffuser	

The following table briefly describes the settings that must be configured before you perform the calculation.

Setting	Description
Start temperature	Select a Start Temperature that is higher than the liquidus temperature of the alloy, in other words, the temperature at which the alloy is completely melted.
Temperature step	Select a Temperature Step. Decreasing the temperature step increases the accuracy, but the default value is usually adequate.
Temperature unit	Select the temperature unit.
Allow BCC> FCC	Select to allow BCC -> FCC transformations in the solidified part of the alloy caused by each of the components specified to be Fast Diffuser . It is recommended that you only select this for steels.
Composition unit	Select the composition unit.
Composition	Specify the composition of the alloy.
Fast diffuser	Select if you want to allow redistribution of this component in both the solid and liquid parts of the alloy.



5. General administration

5.1 Thermo-Calc license information

You can start Thermo-Calc without a valid Thermo-Calc license, but you cannot do any calculations. To use Thermo-Calc, you need a valid standalone **LSERVRC** license file (if you have a standalone installation of Thermo-Calc) or access to license management software (the License Manager on Windows and the License Server on Linux) with a valid network LSERVRC license file (if you have a network client installation).

If you have a network client installation of Thermo-Calc, then you may not be able to do any calculations even if you have access to the licensing server with a valid network license file. This is because other clients who are part of your network installation may have checked out all instances of Thermo-Calc that the network license allows you to run simultaneously.

Also see the *Thermo-Calc Installation Guide* on the website for more information.

To show information about the licenses you have for using Thermo-Calc, from the main menu select **Help>Show License Info**. This opens the License Information window.

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

Figure 11 is an example of the kind of information available for a network client installation. It shows the various license types that the license server makes available (in this case, the license server is *pumbaa.thermocalc.se*).

server por	sking coo st:	5093	233011	5					
icense feat	ures on	license s	erver	numbaa ti	hermocalc :				
Feature	version	number of	davs	sharing	time	site		in	
		licenses	left	criteria	tampering	lice	ense	use	
DIC_FULL	5.000	99	Inf	host	none	192	168.29.*	0	
DIC_FULL	8.000	99	Inf	host	none	192.	168.29.*	6	
test	;	test	-xp-32	2			local		
test	;	test	-cento	os-6-4-32	.thermocal	c.s	:1		
test	:	test	-ubunt	tu-12-04-	64		:1		
test	;	test	-opens	suse-12-3	-64.thermo	cal	:1		
test	;	test	-cento	08-6-4-64	.thermocal	c.s	:1		
test	:	test	-opens	suse-12-3	-32.thermo	cal	:1		
RISMA_FULL	1.000	99	Inf	host	none	192.	168.29.*	0	
RISMA_FULL	3.000	99	Inf	host	none	192.	168.29.*	0	
TC_DLL	5.000	99	Inf	host	none	192.	168.29.*	0	
TC_DLL	7.000	99	Inf	host	none	192.	168.29.*	0	
TC_FULL	5.000	99	Inf	host	none	192.	168.29.*	0	
TC_FULL	7.000	99	Inf	host	none	192.	168.29.*	1	
joha	inj	apol	10				local		

Figure 11 License Information window.

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 is shown. An instance is checked out when an Equilibrium Calculator activity is created, and checked back in when that Equilibrium Calculator is removed. In Console Mode, an instance is checked when a user enters the POLY module and is checked back in when a user exits the POLY module.



For example, you can see that a user *johanj* has checked out a TC_FULL license.

5.2 Editing global defaults

In the **Options** window (select **Tools>Options**) you can globally set general settings for Graphical Mode as well as default settings for any new activities for both the Graphical Mode and Console Mode. The relevant settings for Graphical Mode are briefly described in the following sections.

5.2.1 General

🔺 Opti	ons	
General	Graphical Mode	Console Mode

Setting	Options
Tooltips enabled	Select whether to turn on tooltips information. By default the Tooltips enabled check box is selected. This displays a small text box when you hover the cursor above some buttons or other items.
Localization	To change the GUI language from the Localization list choose English (the default), Swedish, Spanish, German, Russian, Chinese or Japanese.
Look and feel	To change the Look and feel of the GUI layout, choose Windows (the default), Metal, Nimbus, CDE/Motif or Windows Classic.
Database directory	In the Database directory field, specify the path to the directory that contains the data directory. This is where the Thermo-Calc database directory called data is located. Do not specify the path to where the database <i>files</i> are found (that is, in the data directory).
Log level	Select the level and type of information to display in the Event Log window using the Log level slide bar. Choose from a Debug , Info , Warning or Error level of detail.
Check update interval	From the Check update interval list, choose not to check (Don't check , the defaut) or On startup . You can also manually check for updates – choose Help>Check for update .

5.2.2 Graphical Mode - Default Units



Setting	Options
Temperature	Kelvin (the default), Celsius or Fahrenheit
Pressure	Pascal (the default), Atmospheres or Bar
Amount	Mole (the default), Gram, Kilogram or Pound
Composition	Mass percent (the default), Mole percent, Mass faction or Mole fraction
Energy	Joule (the default), Calorie or Electron volt
Volume	Cubic meter (the default), Cubic decimeter or Cubic centimeter
Density	Kilogram per cubic meter (the default) or Gram per cubic meter
Entropy	Joules per Kelvin (the default), Calorie per Kelvin or Electron volt per Kelvin



5.2.3 Graphical Mode – Activities

▲ Options	
General Graphical Mode Cor	sole Mode
Default Units Activities	
🖃 🔲 Default Configurations	
Calculation	Default cal
	Single equ
Plotting	Single equ

There are **Calculation**, **Plotting** and **Tabulation** settings windows.

Calculation: Change the default settings for the Equilibrium Calculator

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



Also see Equilibrium Calculator.

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

Setting	Options
Default calculation mode	Simplified (the default) or Advanced
Default calculation type	Single equilibrium (the default), Property diagram, Phase diagram or Property grid
Single equilibrium and property grid	
Global minimization	The check box is selected by default to ensure that the most stable minimum under the specified conditions is computed.
Max no of iterations	Default is 500
Max grid points	Coarse (2000 grid points, the default), Medium (20,000 grid points), Fine (200,000 grid points), or Custom (set your own number of grid points)
Required accuracy	The default is 1.0E-6
Smallest fraction	The default is 1.0E-12
Approximate driving force for metastable phases	The check box is selected by default
Force positive definite phase Hessian	The check box is selected by default
Control stepsize	The check box is selected by default
Property diagram	
Global minimization	The check box is selected by default to ensure that the most stable minimum under the specified conditions is computed.
Global test interval	Every 10 th eq (the default), Always or Custom
Phase diagram	·
Global minimization	The check box is selected by default to ensure that the most stable minimum under the specified conditions is computed.



Setting	Options
Global test interval	At node points (the default), Every 10 th eq, Always or Custom
Generate starting points automatically	The check box is selected by default
Use inside meshing points	Click to select the check box as required
No of meshes along an axis	The default is 3

Plotting: Change the default settings for any plotted diagrams

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

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



For individual (local) changes to plots see <u>Changing the plot properties</u>. The settings options are the same.

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

Setting	Options
Title	Enter a title. Select Plain text (the default) or LaTeX formatted text.
	Click α button to add symbols. Click a symbol category (for example, Latin characters or Greek and math symbols). Then click to choose the symbol located on the right-hand side.
	When you select LaTeX formatted text you can use the LaTeX math text to enter text. For a list of supported LaTeX commands, see http://www2.ph.ed.ac.uk/snuggletex/documentation/math-mode.html
Title font, Legend font, Label font, Header font	Click Modify to edit the Font Name, Style, Size and Color.
Legend background color, Background color, Canvas color, Border color,	Click Modify to choose a color or enter a specific color.
Label format	Select Plain text (the default) or LaTeX formatted text.
Show anchor	By default, an anchor between the label and the plot point is displayed.
Retain labels (Graphical Mode only)	By default the check box is selected. Plot labels are kept (retained) when plots are updated. It can be applied globally or locally to individual plots.
Show header (Console Mode only)	Click to select the Show header check box to display the basic details about the plot along the top. This includes the date and time the plot is generated, the database used and the properties.
Border width	Choose a plot border width between 1 (thin, the default) and 10 (thick).
Color option	For the plot line colors, choose from the options in the list: Legacy, Printer friendly, JFree chart, Pastel, Medium dark, Bright dark, Vivid or Earth.



Setting	Options
	This option is also available for specific plot lines. To change the color of an individual plot line double-click it in the Results window and use the color palette to define it or enter a specific color.
Line width	For the plot line width, choose from the options in the list. These options are also available for specific plot lines. To change an individual plot line width double-click it in the Results window.
Line type	This option is only available for individual plot lines. To change an individual plot line type double-click it in the Results window and choose an option from the list.
Show data points	Click to select the check box to display the data points on the plot lines. This option is also available for specific plot lines. To show data points on an individual plot line double-click it in the Results window and select the check box.
Data point marker size	Choose the data point marker size between 1 (small) and 10 (large). The default is 3.
Plot Area Size	The Fit the plot area size to the enclosing window option is selected by default. Excluding triangular plots, click Define the plot area size to enter a Plot area height and Plot area width.

Tabulation: Change the default setting for the Table Renderer activity

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

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