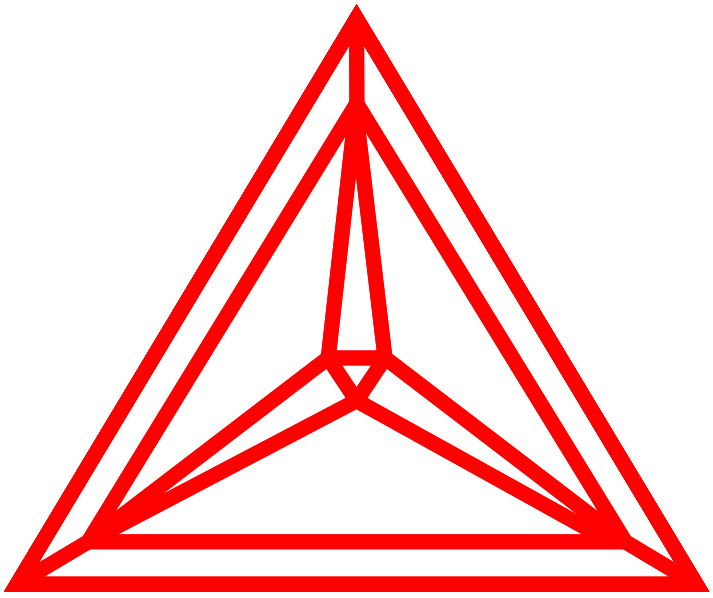

Thermo-Calc

for Windows

Version 5

User's Guide

June 2008

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There may be some minor differences in contents between this Users' Guide and the actual appearance of the program as seen on the screen when running the Thermo-Calc Windows. This is because that some of the contents may need to be updated in the program's on-line help and in the future release of the program. Please visit the Thermo-Calc Software web site (www.thermocalc.com) for any patch (with modifications and/or improvements that have been incorporated into the program and its on-line help), or any amendment that have made to the content of the User's Guides and Examples Books, or to the FAQ lists and other technical information publications.

Acknowledgement of Copyright and Trademark Names:

Availability of This Document:

For the purpose of environment-friendlessness, this Thermo-Calc for Windows Users Guide and all other operational manuals (User's Guides and Examples Books), as well as Reference Lists and other technical documentations, for the TCS-provided software, databases and programming interfaces are provided along the delivered TCS Standard Products CDs and installed on each of designated installation, which can be reviewed and accessed easily and conveniently. If desired and preferred, a user can locally print such a manual but it is only for the purpose of the user's internal use.

To make manual updating more prompt and efficient, the later manual revisions or additions will be made available on the Internet. Our users may therefore download such revised documents from our web site www.thermocalc.com.

Contents

1 WHAT IS THERMO-CALC FOR WINDOWS?

Thermo-Calc for Windows, also known as Thermo-Calc, is the graphical user interface version for Windows of the Thermo-Calc software. Thermo-Calc for Windows offers material scientists and process engineers a user-friendly and intuitive way of performing advanced thermodynamic calculations. Multicomponent phase diagrams and property diagrams can be obtained by a few clicks in a couple of windows.

The Thermo-Calc for Windows software is the fastest and most efficient way of performing thermodynamic calculations for beginners and occasional users. The current version is number 5, which is continuously developed to, and beyond the functionality in the classic version of Thermo-Calc.

Thermo-Calc for Windows uses the same thermodynamic databases as Thermo-Calc Classic, which has been in commercial use since 1984 and today is internationally renowned. All databases from Thermo-Calc Software contain reliable and carefully assessed data available for a wide range of materials and applications.

Thermo-Calc for Windows is currently available for Windows 2000/XP/VISTA.

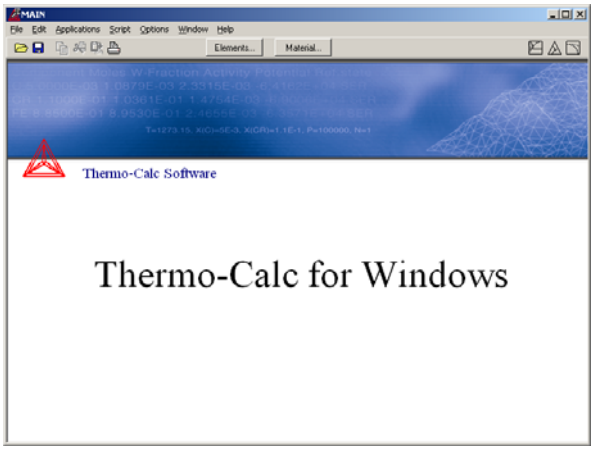
2 HOW TO USE THIS MANUAL

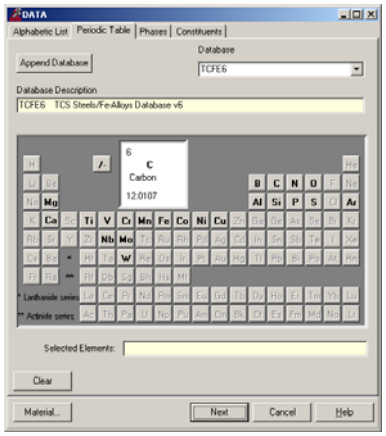
This manual describes the functions and commands of Thermo-Calc for Windows, and the software require an understanding of thermodynamics. Examples of problems solved with Thermo-Calc are described in the Examples Book.

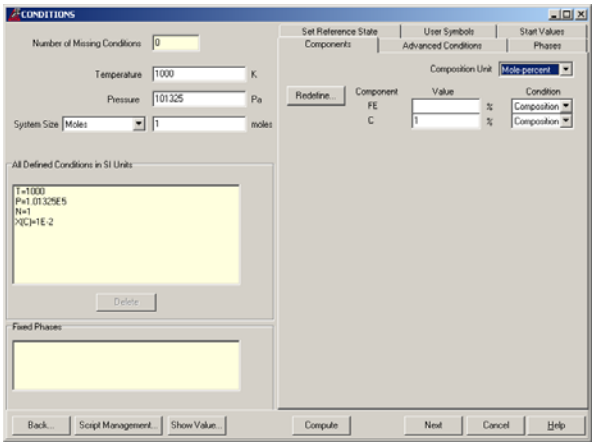
3 INSTALLING THE SOFTWARE AND DATABASES

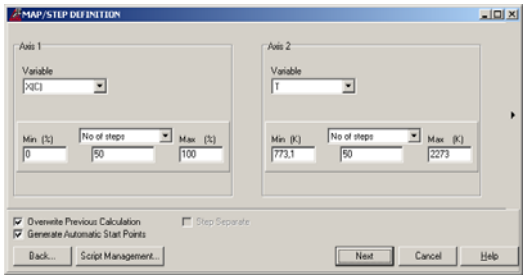
The software comes with an installation guide in the CD-box alternatively on the installation CD as a PDF-file.

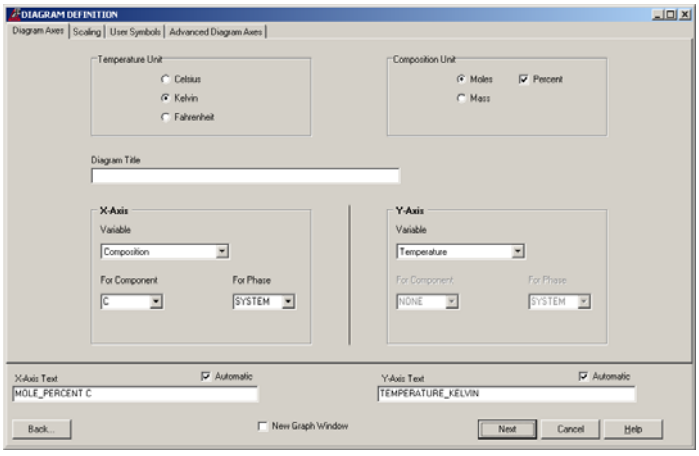
4 MAIN WINDOWS

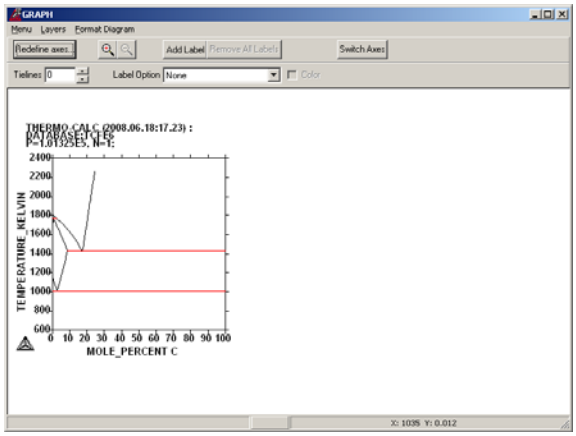






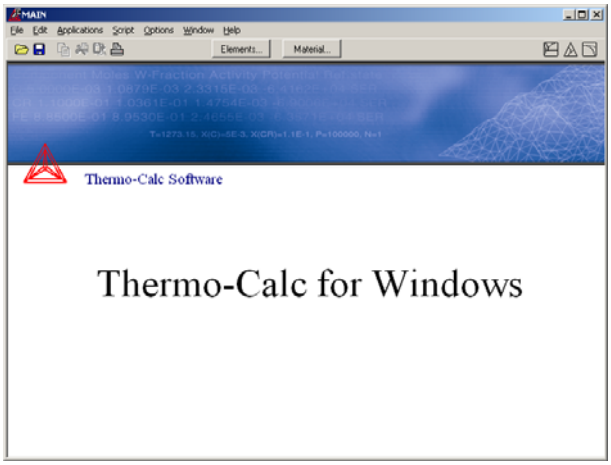






5 THERMO-CALC MAIN

This window is always open when Thermo-Calc is running. Most of the windows within the program can be reached from here. All of the equilibrium information is shown and manipulated with this window: opening a former equilibrium, computing a new one, or saving the current one.



Menu bar

File	Open a preexisting file, save a file, or exit the program.
Edit	Undo, Cut, Copy, Paste, Delete, Select all text in a window.
Applications	Start an application; Binary, Ternary phase diagrams, or a Scheil simulation.
Script	Script Management or Run Script.
Options	Settings for Output, Units, Default Temperature for Step and MAP, settings for Equilibria Calculation, and Default Materials Folder.
Window	Choose which of the Main windows that will be shown, and choose what is shown in the THERMO-CALC Main window.
Help	Help contents, THERMO-CALC version information, the THERMO-CALC Software System document, the THERMO-CALC User's Guide (this document), the THERMO-CALC Example Collection and the Thermo-Calc website.

Toolbar

Elements	Opens the THERMO-CALC DATA window where a system can be set up by choosing elements, phases and a database. See section 6.
Material	Opens the THERMO-CALC Select Materials window where a material can be chosen from the materials database. See section 7.
	Define a binary system and calculate a binary phase diagram, Gibbs energy curves, Activity curves or Phase fraction diagram. See section 8.1.
	Define a ternary system and calculate isothermal section, monovariant lines or liquidus projection diagrams. See section 8.2.
	Simulate a solidification processes using the Scheil-Gulliver model. See section 8.3.

6 MAIN: ELEMENTS MODULE

This chapter describes the features of the MAIN WINDOWS.

6.1 THERMO-CALC DATA

This window has four tabs:

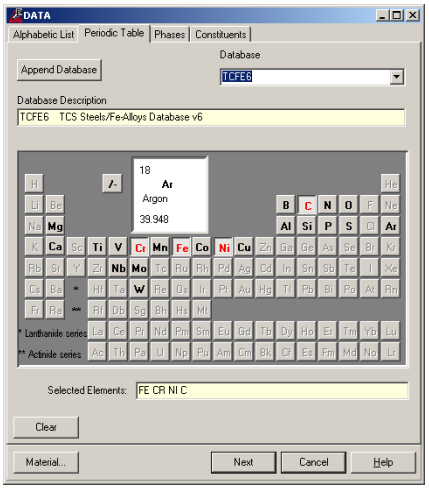
- Alphabetic List
- Periodic Table
- Phases
- Constituents.

The Periodic Table is first to appear after clicking the Elements key on the toolbar in the THERMO-CALC MAIN window.

On all tabs

Material	Opens the SELECT MATERIAL window in the Materials Module, see section 7.1, were you can get predefined materials to the DATA window.
Next	Go to the next MAIN WINDOW.
Cancel	Close window without remembering selection/changes.
Help	Show the THERMO-CALC Help page regarding present window / tab.

6.1.1 TAB: Periodic Table



In this window the available elements within the selected database are presented on the periodic table. The system to study may be defined here.

In this particular case the TCFE6 database has been chosen and the periodic table shows in bold character all the elements within the TCFE6 database.

Toggle a particular element by left clicking on it. It turns red when selected. The gray elements are not included within the database and can not be chosen or shown information for. Move the mouse over a particular element to see its name, atom number, and atomic mass in the square field.
Here have been selected the four elements Fe, Cr, Ni, and C. Press the Next button to proceed to the THERMO-CALC Conditions window (see section 6.2).

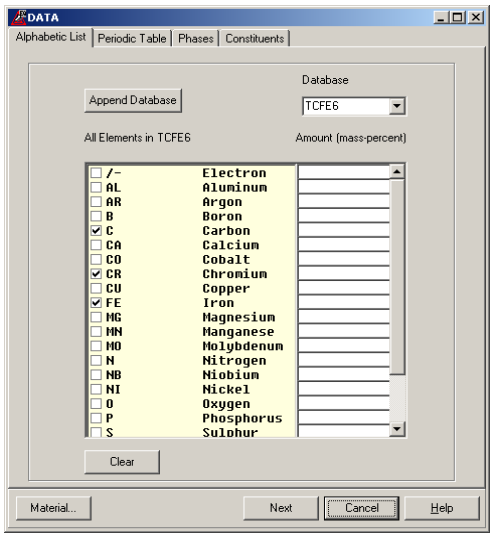
Functional Keys

Append Database	If desired, click on “Append Database” to append another database with the same element selection (you need to then choose the appended database name). (See 6.6.3)
Clear	Deselect all elements

Field

Database	Here the database is chosen

6.1.2 TAB: Alphabetic List



In this window the available elements within the chosen database are displayed in alphabetic order. If preferred, the studied system can be defined here. Check the check box in front of the desired element to select it.

In the right column the amount of the element may be entered. This amount is converted to a condition in the Condition window when pressing *Next*.

In this particular case the TCFE6 database has been chosen and the field shows all the elements within the TCFE6 database. Three elements, C, Cr and Fe, have been chosen. No amount is set.

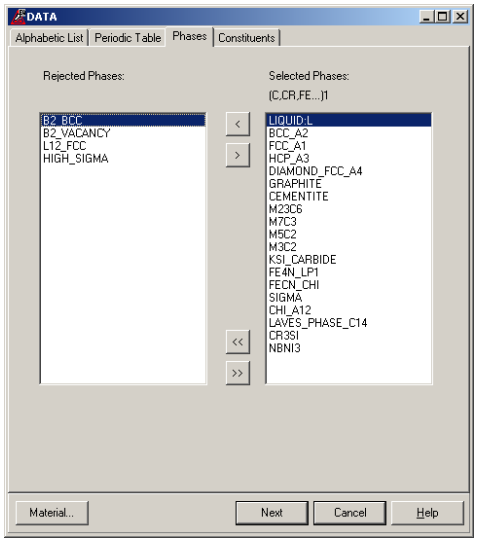
Functional Keys

Append Database	If desired, click on “Append Database” to append another database with the same element selection (you need to then choose the appended database name).
Clear	Deselect all elements

Field

Database	Here the database is chosen

6.1.3 TAB: Phases



In this window it is possible to specify the phases that the calculation will be based upon by selecting phases or rejecting phases.

With the single arrow keys a phase can be transferred to either a selected or rejected state. By using the Shift and Ctrl keys multiple phases can be transferred.

The double arrow keys transfer all of the phases to the other field.

In this particular case the B2_BCC, B2_VACANCY, L12_FCC and HIGH_SIGMA phases will not be considered in the calculation. All of the phases listed in the Selected Phases field will be retrieved from the database and considered in the calculation.

Selecting a phase in the “selected phase” list will show the structure of this phase above the list.

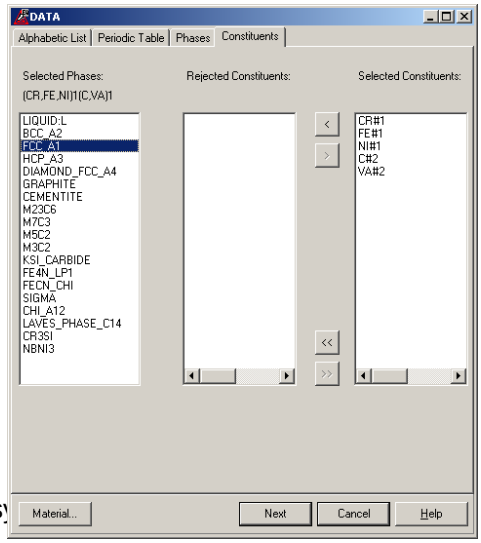
Fields

Rejected Phases	Shows the rejected phases omitted from the chosen system.
Selected Phases	Shows the phases that the calculation will be based upon.

Functional Keys

Single Arrows	Use the single arrow keys to transfer (reject or restore) phases between the two fields. First *click* on the phase to select it, and then on the arrow key to transfer the phase. The Shift and Ctrl keys can be used to select multiple phases.
Double Arrows	The double arrow keys transfer all of the phases to the other field.

6.1.4 TAB: Constituents



This window identifies the constituents, for a phase specified in the list of selected phases.

Using the arrow keys it's possible to reject or select constituents for the specified phase.

In this particular case the constituents in the FCC_A1 phase are displayed. The FCC_A1 phase contains the elements Cr, Fe and Ni in one sub-lattice, #1. Another lattice, #2, contains the interstitial C and VA (vacancies).

Mark the phase by a left click, select the constituents to change status for and then change status pressing the arrow.

Fields

Selected Phase Shows the selected phase of the particular sy

Rejected Constituents List rejected constituents

Selected Constituents Identifies the elements or species within the selected phase to be used in the calculation. VA denotes vacancies.

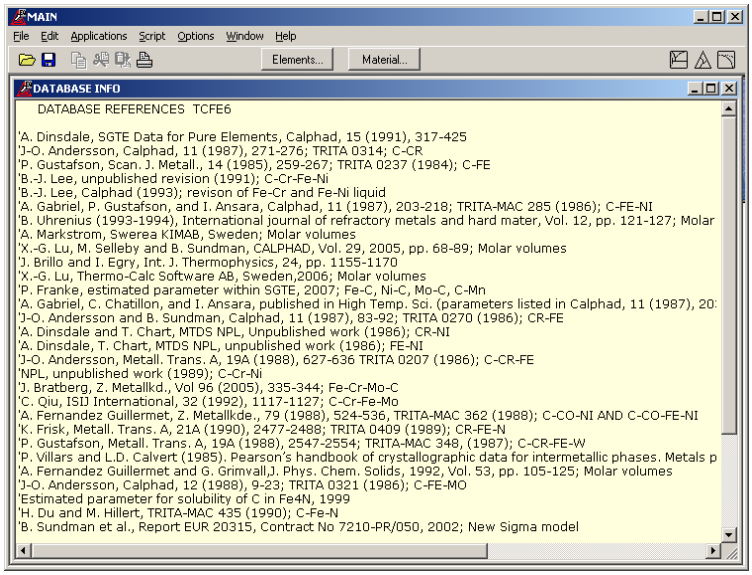
Functional Keys

Single Arrows Use the arrow keys in order to transfer a selected constituent of a phase to the other state.

Double Arrows The double arrow keys transfer all of the constituents to the other field.

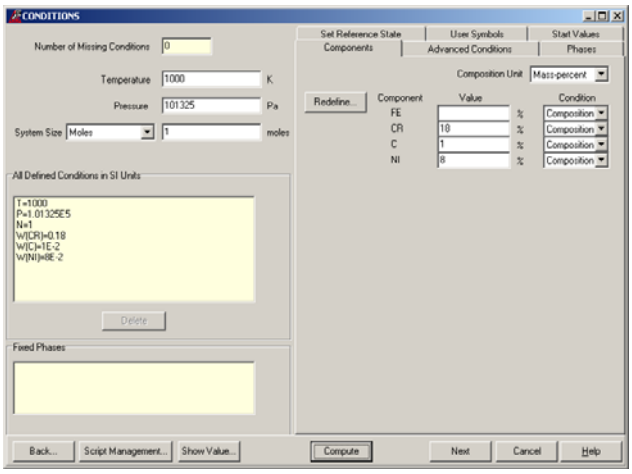
6.2 DATABASE INFO

After pressing the button NEXT in the THERMO-CALC DATA window, the references used for the chosen system in the selected database are listed in a THERMO-CALC MAIN sub-window.



6.3 THERMO-CALC CONDITIONS

In this window the conditions for the equilibrium may be specified.



After specifying the conditions for the equilibrium, you may perform a calculation either by pressing the “Compute” or “Next” button. However, first the number of missing conditions must have been reduced to zero.

In order to calculate a property diagram or phase diagram, press the “Next” button.

The temperature condition unit is per default in K but can be changed using the THERMO-CALC UNITS window (in the THERMO-CALC Main window) to C or to F.

The “Script Management” button will take you to the THERMO-CALC SCRIPT MANAGEMENT window, where you can store the current setup as a user defined script.

Fields

Number of missing conditions	Show the number of missing conditions. Click in field to update it.
Temperature	Enter the selected temperature for the system
Pressure	Enter the selected pressure for the system
System Size	Choose the selected unit and enter the amount for the system
All defined conditions	Shows the defined conditions in SI units
Fixed Phases	Lists the fixed phases, if any. To modify this use the Phases Tab.

Functional Keys

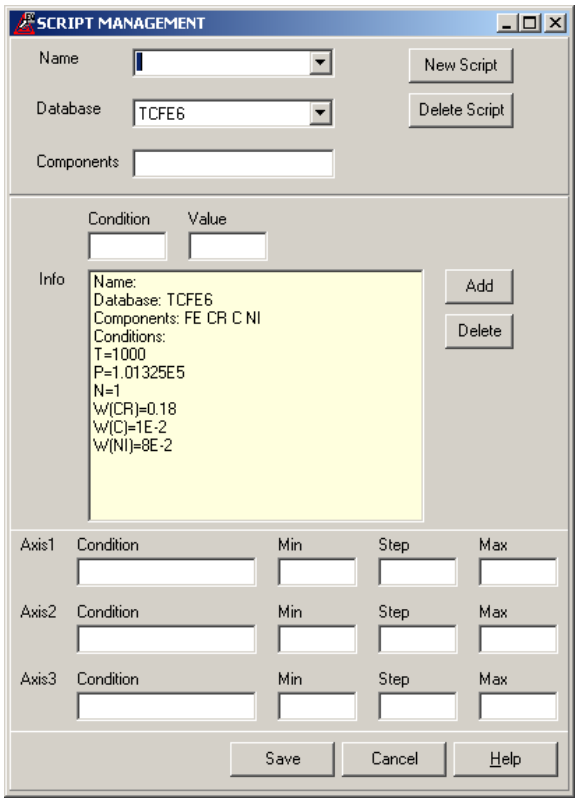
Script Management	Clicking the “Script Management” button will open the SCRIPT MANAGEMENT window. See 6.3.1.
Show Value	Clicking the “Show Value” button will open the “Show Value” window. See 6.3.2.
Compute	Press to apply the conditions and calculate the equilibrium without closing the CONDITIONS window.
Next	Perform the calculation, like Compute above, and go to the THERMO-CALC MAP/STEP DEFINITION window.
Cancel	Close window without remembering selection/changes
Help	Show the THERMO-CALC Help page regarding present window/tab

Functional Tabs

The functional tabs are described under section 6.3.4.

6.3.1 KEY: Script Management

The alloy script uses the TCFE6 database. The weight-fraction of C, CR, MN is 0.0002, 0.22 and 0.012. Temperature is 1000K, Pressure is 100000 Pa, total number of moles is 1. More conditions must be added before equilibrium can be calculated or a graph plotted. The Script Management window may also be opened from the Scripts menu in the THERMO-CALC Main window. For more information about how to run the created script file see the THERMO-CALC RUN SCRIPT page.



Fields

Name	Chose or Rename an already-present script.
Database	Edit what database to use in chosen script.
Components	Type in an element or species to be part of the alloy and then press the Add button.
Conditions / Value	Enter a condition in POLY-3 syntax, for example W(CR). Enter the value of the condition in the Value field, for example 0.18, and click the Add button.
Info	Lists the database, elements, and conditions already designated.
Axis / Conditions	Specify the conditions to be used as variables for the axis. Specify the minimum values, the maximum step sizes, and the maximum values of the conditions. An axis condition is not compulsory.

Functional Keys

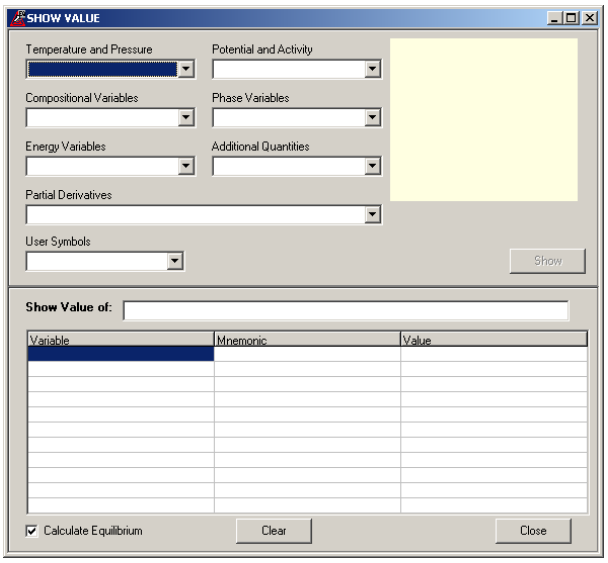
New Script	Make a new script.
Delete	Delete an old script.
Add	After entering a condition, press “Add” to add it.
Delete	Select a condition and click “Delete” to remove it.
Save	Press to save the script to file.

6.3.2 KEY: Show value

Choose the predefined Variable to be shown from one of the eight fields in the top and there after pressing the "Show" button. If selection of a phase, specie, component, or normalization is required they are shown in the top right field. Enter this symbol to the list of shown variables by pressing the "Show" button.

Alternatively enter the expression of the symbol to be shown in the *"Show value of:"* field, enter it to the list of shown variables by pressing the "Show" button.

If the *"Calculate equilibrium"* check box is checked an equilibrium calculation is performed to ensure that the correct value is displayed. This implies that the equilibrium conditions must be correct before showing the value of a symbol. See also 6.5.4



Fields

Show value of: Shows the expression for an already-entered (or predefined) symbol name after you selected it. Here you may specify/edit an expression for the property you want to view.

Functional Keys

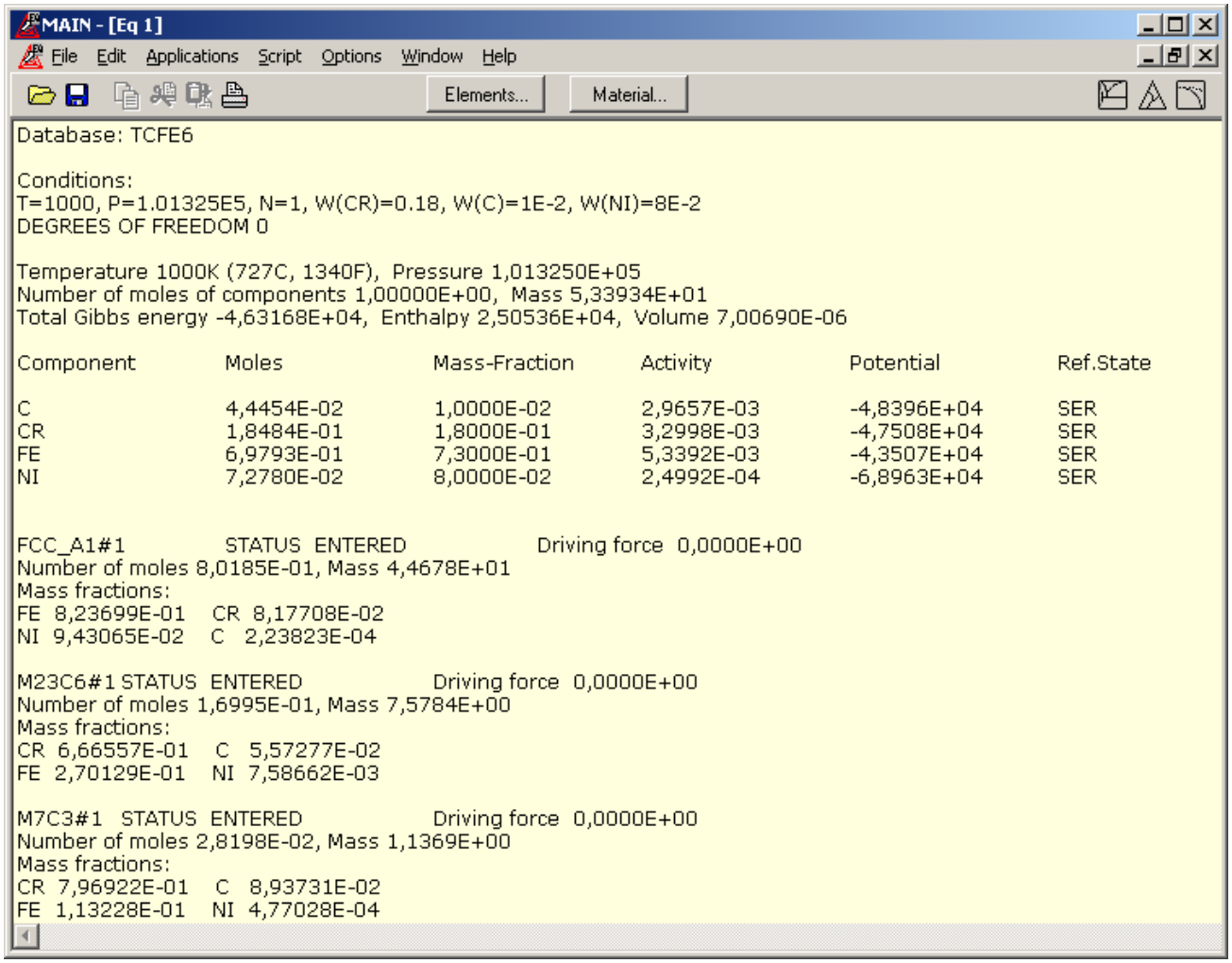
Show — Enter the chosen or defined variable or expression from the *"Show value of:"* field into the Variable list.

Clear — Remove all Variables in the Variable list.

Close — Close window saving Variable list.

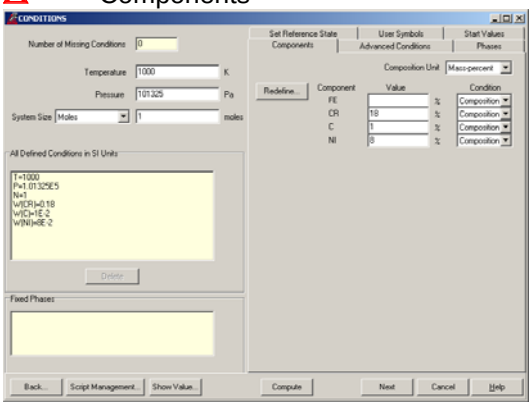
6.3.3 KEY: Compute Equilibrium

After a single equilibrium calculation some info about the equilibrium properties are shown in the lower part of the MAIN window.
The used database
The initial conditions for the calculation from the THERMO-CALC CONDITIONS window.
Temperature and Pressure
Moles of components, Mass of system
System Composition, activity and potential all in components.
Fore each stable or dormant phase
Name, Status, Driving force
Number of moles, Mass
Composition of phase

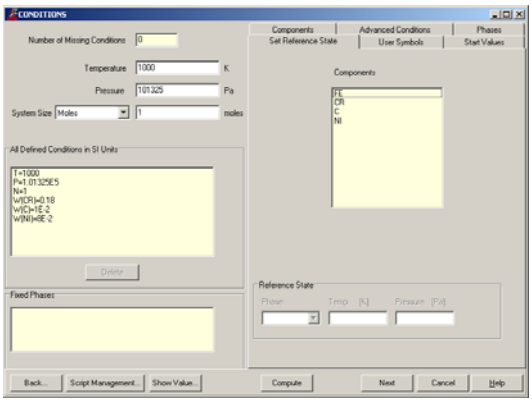


6.3.4 TABS

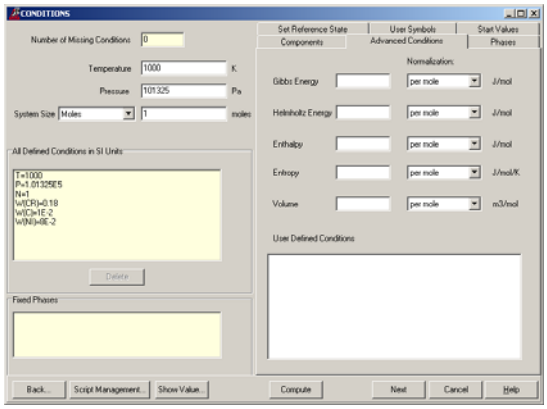
Components



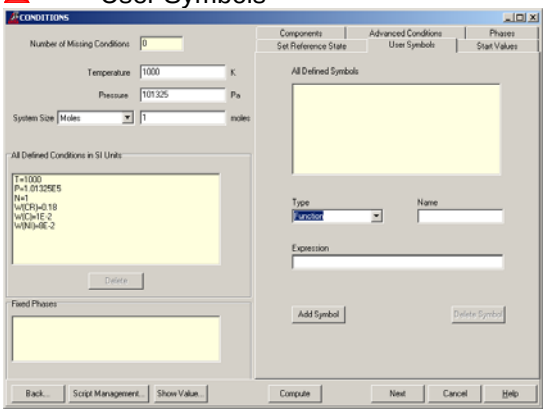
Set Reference State



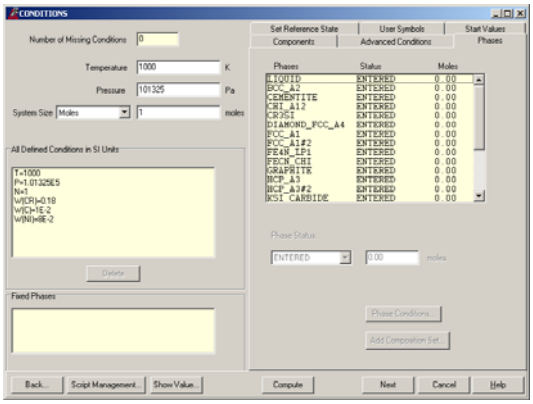
Advanced Conditions



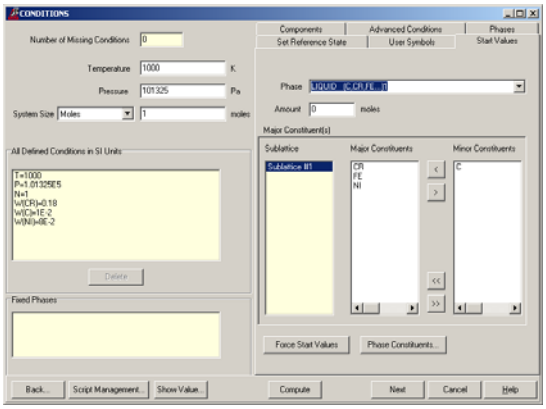
User Symbols



Phases

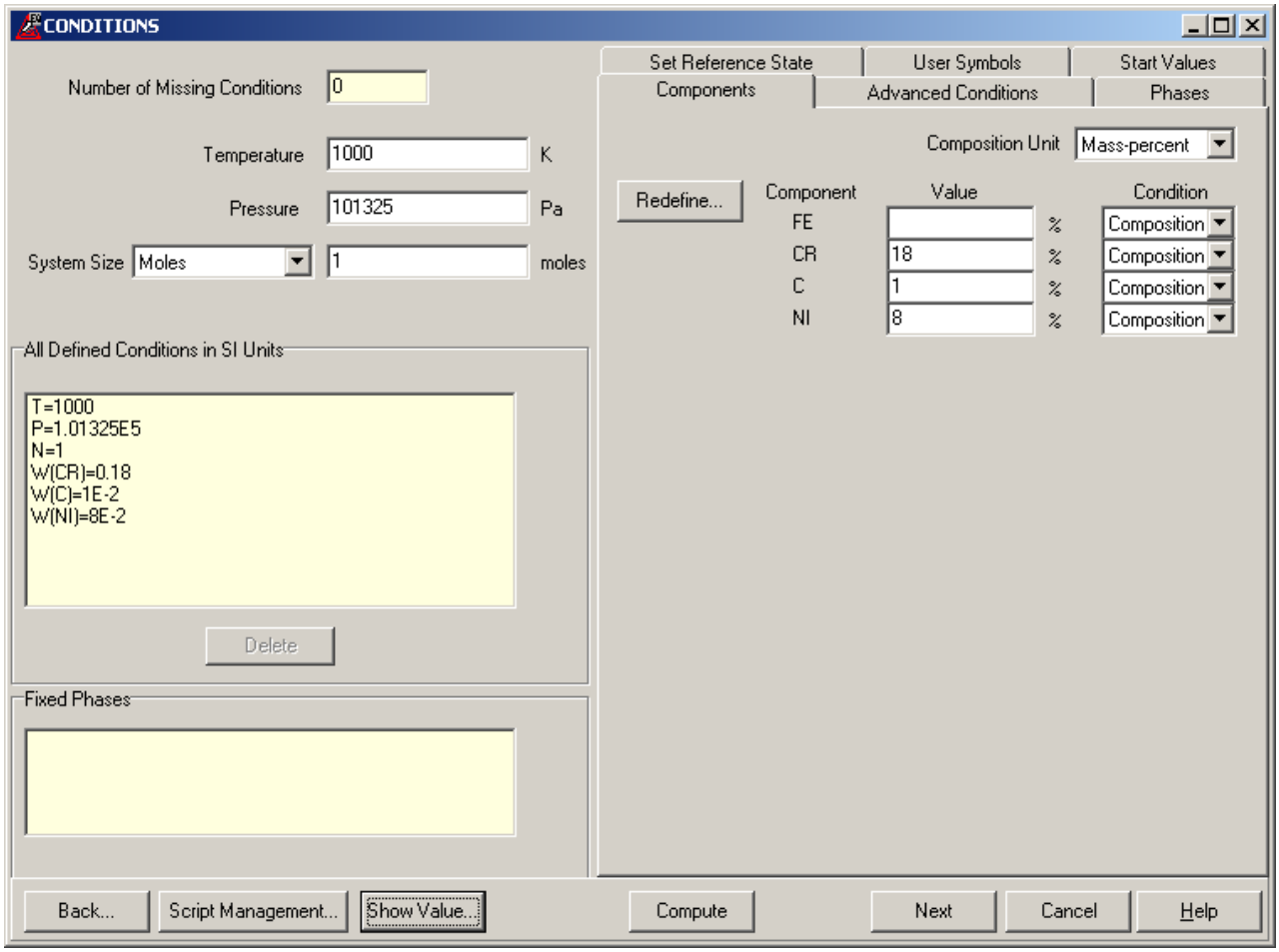


Start Value



6.3.4.1 TAB: Components

Define components and set conditions for components



Fields

Composition Unit — Choose the composition unit for the listed components. Choose among mass, mass-fraction, mass percent, moles, mole-fraction, mole-percent.

Value / Condition — Type in the value of the condition. Choose type of condition among composition, activity, and chemical potential. Leave empty if no condition is wanted.

Functional Keys

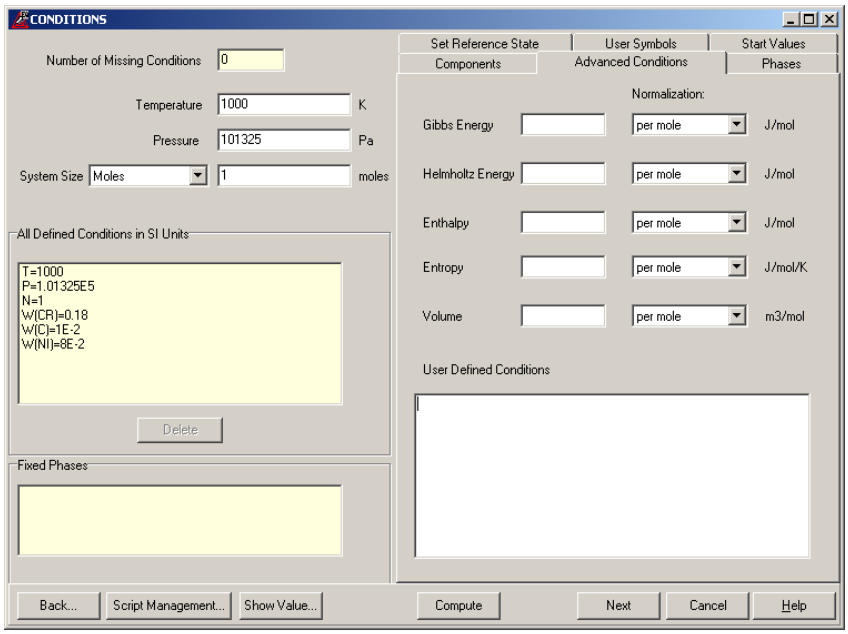
Redefine — Change the set of components to suit the needs of the particular calculation. For example, when calculating along the section from CrO2 to Fe2O3, it may be useful to redefine the components to CrO2, Fe2O3, instead of Cr and Fe. The number of components must still be the same; components cannot be removed or added. Redefining the components resets the conditions and new conditions may have to be specified. The new set of components must be a linear combination of the system elements, and they should not be linearly dependent.

6.3.4.2 TAB: Advanced Conditions

In this window the user may enter conditions as a function of several state variables.

Also in this window, conditions on any extensive property like G, H, S etc can be set per mole of components in the system, per mass in the system, per volume in the system or for the whole system (current amount). Setting the property per volume can only be done if the database has pressure dependence.

Note, when entering state functions it may be necessary to remove previously defined conditions, in order to maintain zero degrees of freedom



Fields

Gibbs Energy

Helmholtz Energy

Enthalpy

Entropy

Volume

Set the properties (Gibbs Energy, Helmholtz Energy, Enthalpy, Entropy, Volume) to specific values to define the initial conditions of the system.
These options are rarely used when defining a system's conditions.

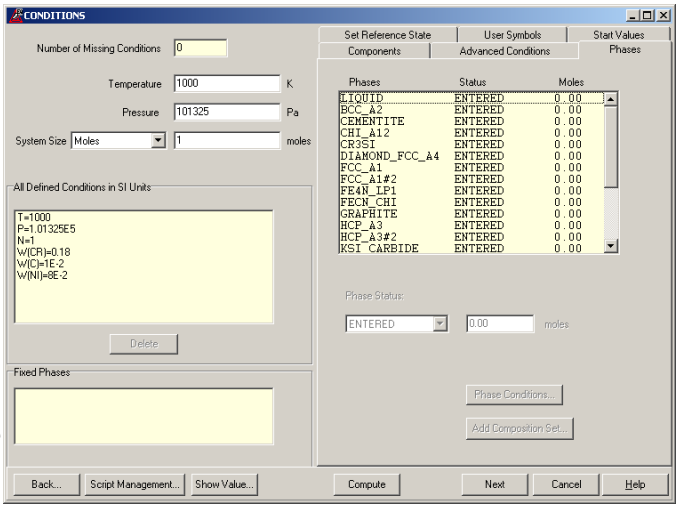
Normalization

User Defined Conditions

Define your own conditions in POLY-3 format. For example, conditions that involve two or more state variables can be entered here. Input these conditions in TCC format, for example W(Cr)-10*W(C)=0 to assure that for every gram of C, there are 10 grams of Cr in the system.

6.3.4.3 TAB: Phases

Under this tab the status of one or more selected phases can be changed. The default status is ENTERED, which means that the phase is included in the calculation and it will be stable if that minimizes the total energy. A phase that is SUSPENDED will be ignored. It is possible to calculate a metastable equilibrium by suspending a stable phase. A DORMANT status means that the phase is not considered in the calculation, but the driving force for precipitation is calculated. A FIXED status means that it is a condition that the phase must be stable. Setting the status FIXED for a phase reduces the number of missing conditions by one.



Fields

Phase / Status / Moles	Shows all phases in the system their status and present amount of formula unit of the phase
Phase Status	Select a phase by clicking on it and then change its phase status between ENTERED, FIXED, DORMANT, or SUSPENDED. If ENTERED you may set a start amount, and if FIX you set a condition for its amount in moles of formula units

Functional Keys

Phase Conditions	Clicking the “Phase Conditions...” button will open the PHASE CONDITIONS window where phase property conditions are set. Note that although more than one phase can be simultaneously selected in the Phases field, phase property conditions can be set for only one phase at a time. See section 6.3.7.1.
Add Composition Set	Clicking the “Add Composition Set…” button will open the COMPOSITION SET window in order to add a composition set for a selected phase that may have a miscibility gap. This button is activated when a phase is marked in the Phases field, so that the added composition set is for that specific phase (e.g., BCC_A2#2 for BCC_A2). See section 6.3.7.2.

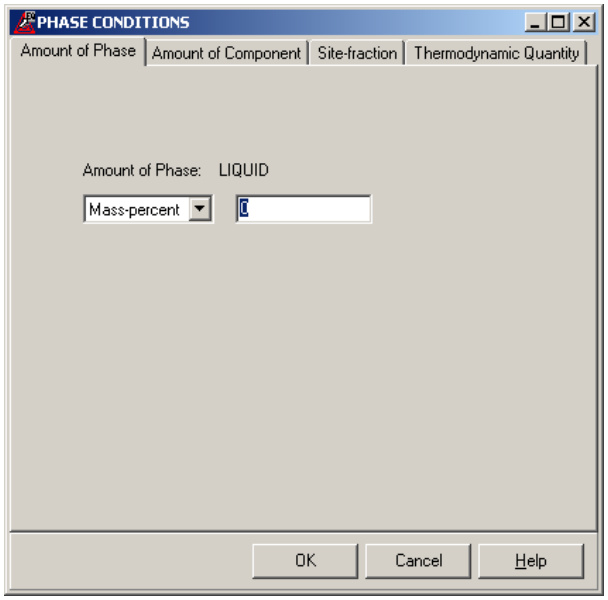
6.3.4.3.1 PHASE CONDITIONS

Set the phase property conditions of a specified phase in the THERMO-CALC PHASE CONDITIONS window. If you are so advanced that you want to use these conditions, you do not need any help. However, try right mouse clicking on the buttons or pressing F1 in the fields…

Any setting of phase property condition made on the current window will be promptly translated and updated, and simultaneously shown up on the All Defined Conditions field on the THERMO-CALC CONDITIONS window.

TABS

- Amount of Phase
- Amount of Component
- Site-fraction
- Thermodynamic Quantity



6.3.4.3.1.1 TAB: Amount of phase

The amount of a phase can be set as a condition in the initial equilibrium calculation.

It is recommended to do this in the THERMO-CALC CONDITIONS Phases window by using the status FIXED instead.

Select the appropriate unit (moles, mole-fraction, mole-percent, mass, mass-fraction, mass-percent, volume, volume-fraction) and type in the particular amount.

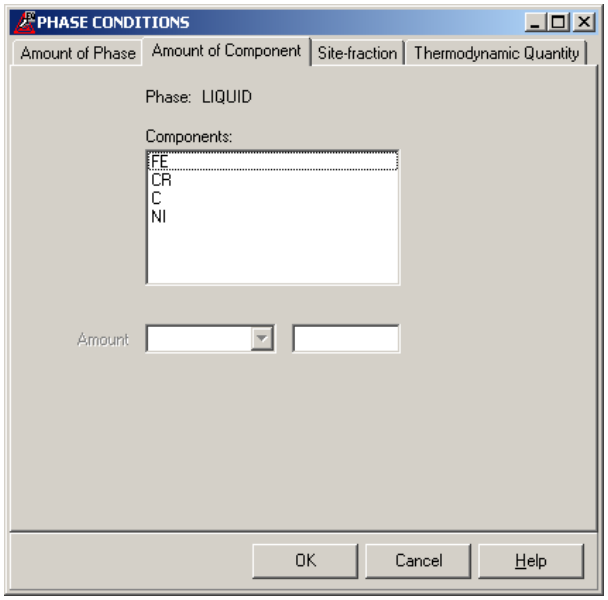
Fields

Amount of Phase / Value Select the unit and enter the value

6.3.4.3.1.2 TAB: Amount of Component

The compositions given in the THERMO-CALC CONDITIONS window are overall conditions. In some cases, it may be interesting to calculate with the composition of a specific phase as a condition instead. Such conditions can be specified using this window.

Note: Equilibrium calculations may fail if the conditions are not logical or if the conditions cannot be fulfilled. For example, if BCC_A2 cannot exist at the specified composition, the equilibrium calculation will fail.



Fields

Component	Choose the component to set the amount.
Amount / Value	Select the unit (moles, mole-fraction, mole-percent, mass, mass-fraction and mass-percent). Set the amount for a selected component in a phase.

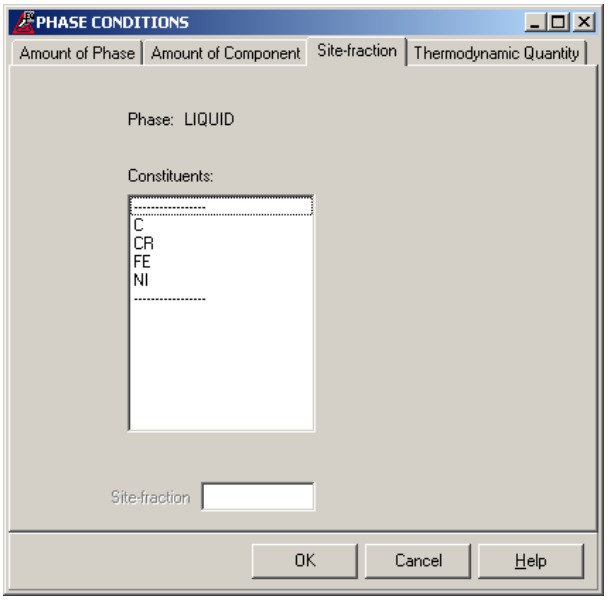
6.3.4.3.1.3 TAB: Site-fraction

The constitution of a phase is expressed using site-fractions.
For example, Y(phase,species#sublattice).

Using this window it is possible to set a condition on the site-fraction of a certain constituent. Simply select a constituent and specify a certain value.

Dashed lines divide the different sub-lattices.

Note that VA denotes vacancies.

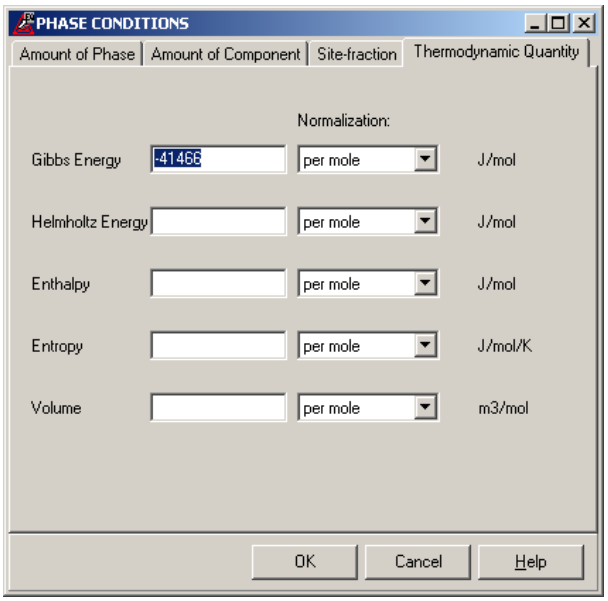


Fields

Constituents	Choose the component to quantify.
Site-fraction	Quantify the amount for the site-fraction.

6.3.4.3.1.4 TAB: Thermodynamic Quantity

Using this window it's possible to set the amount for a particular extrinsic variable per mole of components of the phase, per mass of the phase, per volume of the phase or for the current amount of the phase.



Fields

Gibbs Energy
Gibbs Energy
Helmholtz Energy
Enthalpy
Entropy
Volume

+ Normalization — Specify the value for the thermodynamic quantity

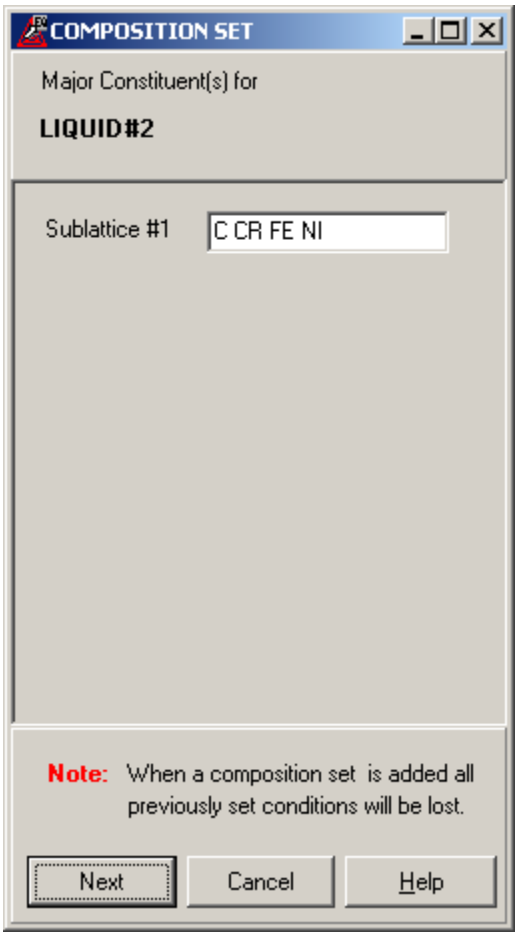
6.3.4.3.2 COMPOSITION SETS

Clicking the Add Composition Set key will open the COMPOSITION SET window in order to add a new composition set for a selected phase that may have a miscibility gap. This button is activated when a phase is marked in the Phases field, so that the added composition set is for that specific phase (e.g., BCC_A2#2 for BCC_A2).

In some cases, it is possible that two phases with the same structure but different compositions are in equilibrium. This is described as a miscibility gap in a single-phase system. In order to calculate such equilibrium, it is necessary to introduce the same number of composition sets for the phase as simultaneously stable compositions.

By pressing the Add Composition Set button in the CONDITIONS window an additional composition set can be created.

If global optimization is enabled composition sets are created when needed and this feature is rarely useful.

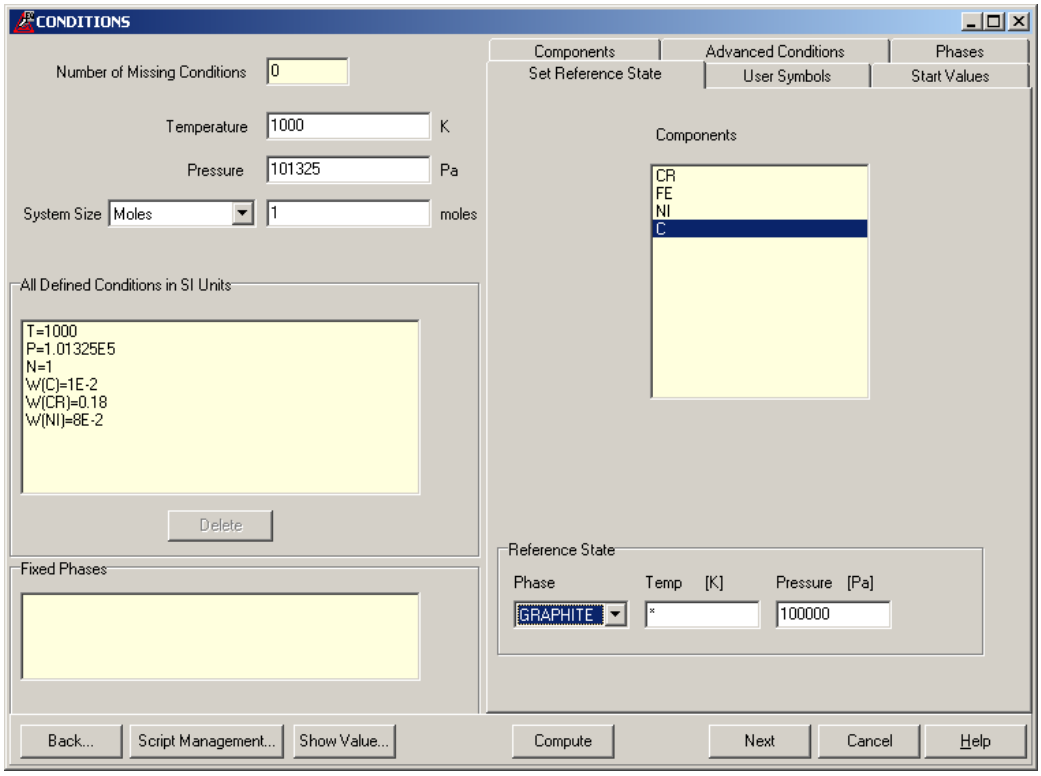


Fields

Sublattice #1 Specify the MAJOR constituents on the different sub-lattices for the added composition set. All the constituents of a sub-lattice are not necessarily major constituents for a created phase#2! The given information is used when setting start constitution.

Sublattice #2 Same as above

6.3.5 TAB: Set Reference State



The reference state for a component is determined by the database. For each component the data is referred to a selected phase, temperature and pressure.
The reference state for a component is important when using activities, chemical potentials and enthalpies. By default these are computed relative to the reference state defined in the database.

In this window the user may specify other reference states for the components.

In this particular case the reference state for C has been changed from being SER (Stable Element Reference) that is graphite but at 298 K to Graphite at any T of calculation.

Select a component and set Reference State for it by selecting Phase, Temperature and Pressure.

Field

Components — Identifies the components of the system. Mark one to check/change the reference state.

Phase: — Any phase in which the component can be the single constituent can be selected as the reference state.

Temperature: — If a phase is specified rather than SER, then a temperature can be selected. "*" prescribes the reference state to be the temperature that is used in the actual calculation.

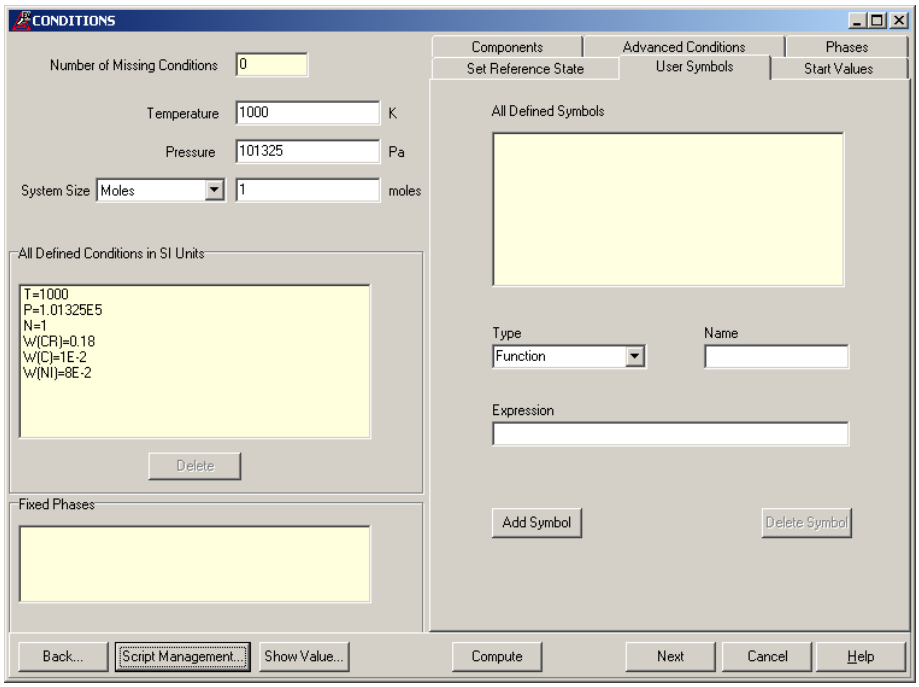
Pressure: — If a phase is specified rather than SER, then a pressure can be selected. The default pressure is 105 Pa (1bar).

6.3.6 TAB: User Symbols

Under this tab the user may enter own symbols.

A symbol may be either a constant, e.g. a numeric value, or an expression of state variables. For more information regarding state variables see chapter 2.5 and 2.6 in the “Thermo-Calc Software System” manual.

A symbol can typically be used as a condition in the calculation, e.g. if a constant P0=1e5 is entered and P0 is set as a condition, or in order to evaluate some function of state variables after a stepping operation.



Fields

All Defined Symbols — This field display all the symbols already defined.

Type — **Constants**: are just a means of using a name for a numeric value.
Functions: are expressions of state variables or other functions. These expressions are saved, and whenever a function value is requested all functions are evaluated.
Variables: are similar to functions because they can also be expressions of state variables. However, contrary to functions, they will only be evaluated when they are entered or if they are explicitly called upon.
Tables: are made by entering functions or variables defined in THERMO-CALC by default or previously entered by the user and separated by a space or a coma.

Name — Your name for the symbol to be entered.

Expression — Enter a numeric value, or an expression of state variables or other functions.

Functional Keys

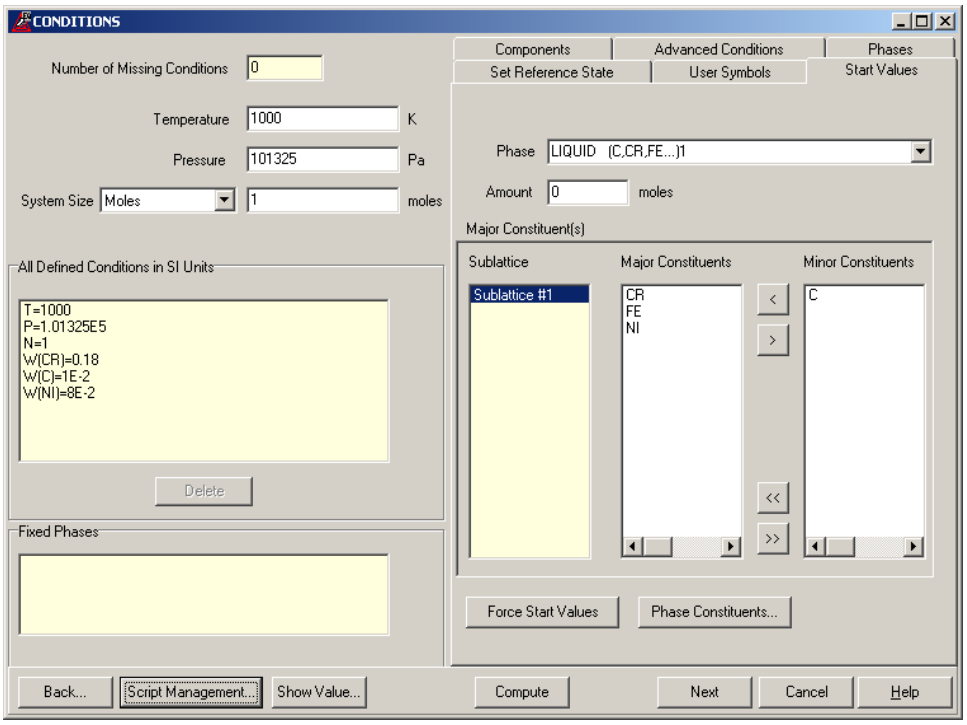
Add Symbol — Add the expression defined to the symbols list.

Delete Symbol — Delete the marked symbol(s) in the “All Defined Symbols” field.

6.3.7 TAB: Start Values

If a calculation, where global optimization is not used, fails to converge it might help to provide the program with suitable start values.

The first attempt is to specify the major and minor constituents on the different sub-lattices for one or several of the phases. If the program still fails to find the correct equilibrium, continue by quantifying the constituents for each phase by pressing the “Phase Constituents” button. The button “Force Start Values” will reset all the start values to “fresh” ones. This can be useful if e.g. erroneous conditions have been used causing unrealistic start values.



Fields

Phase	Selected phase for which start values can be provided.
Amount	The amount of the selected phase can also be specified as a start value.
Major Constituent(s)	
Sublattice	Showing the sublattices
Major Constituents	Suggested major constituents on the selected sub-lattice.
Minor Constituents	Suggested minor constituents on the selected sub-lattice.
Arrow	Use the arrow keys to transfer (reject or restore) constituents between the two fields
Double Arrow	Use the double arrow keys to transfer (reject or restore) all marked constituents between the two fields

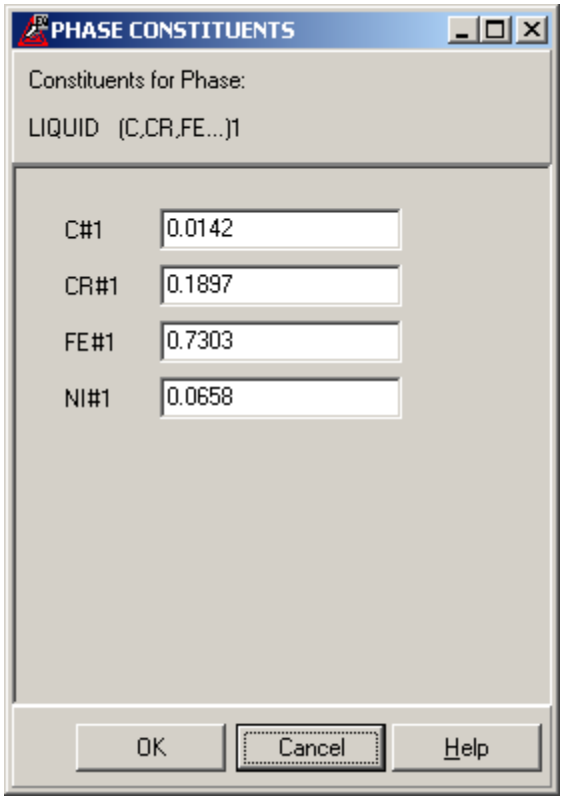
Functional Keys

Force Start Values	*Click* the Force Start Values button to automatically set all the start values for the selected phase, including its Amount, and the Major Constituents on each sublattice in the phase.
Phase Constituents	This key allows the user to manually specify the start values for the constituents in the selected phase by opening the window PHASE CONSTITUENTS.

6.3.7.1 WINDOW: PHASE CONSTITUENTS

In extreme cases when the global minimization is turned of and if the program fails to calculate equilibrium the user can help the program by providing explicit start values. If the provided start constitution is close enough to a global minimum, then the calculation should converge to the correct equilibrium.

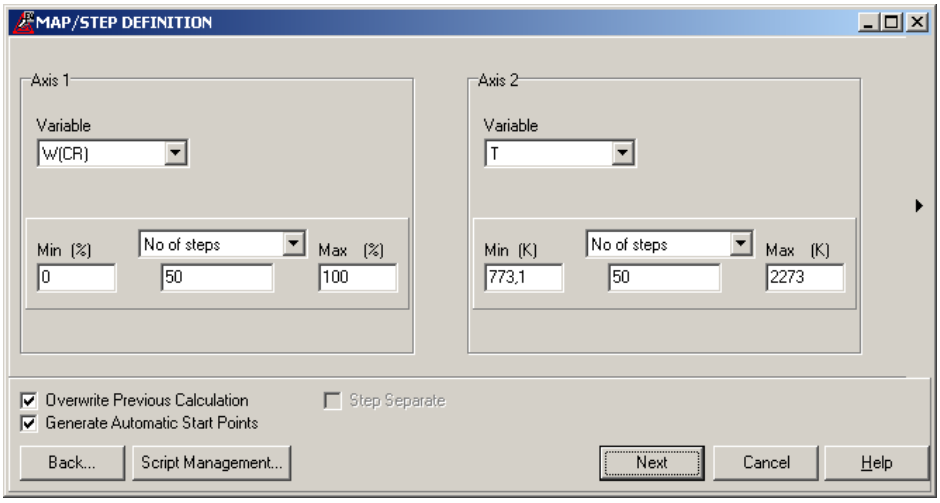
Click the Phase Constituents key to open the THERMO-CALC PHASE CONSTITUENTS window, to specify the start values for all constituents in the selected phase. Once the THERMO-CALC PHASE CONSTITUENTS window has been opened, you can select any phase on the Set Start Value tab of the THERMO-CALC CONDITION window to specify the start values of its constituents, till the THERMO-CALC PHASE CONSTITUENTS window is closed after clicking on its OK button.



Fields

Constituents for Phase	Specify a start value for one or several of the constituents in the selected phase.

6.4 MAP / STEP DEFINITION



In this window, it is possible to define a MAP and STEP calculation.
A property diagram is calculated in a STEP calculation with one independent axis variable and the variable for the other axis set to None.
A phase diagram is calculated in a MAP calculation with two independent axis variables. The software will then map the phase diagram lines within the axis limits. It is the case with the settings above.

Fields

Variable	Set the property to vary over the axis. Choose between: None, T, P, Mass fraction (percent), N, Temperature, Pressure, Amount, Amount of Phase, Activity, Potential, Gibbs energy, Enthalpy, and Entropy.
Min / Steps / Max	Set: - Minimum value for the map/step calculation. - Number of steps or the stepping size of the calculation. - Maximum value for the map/step calculation.

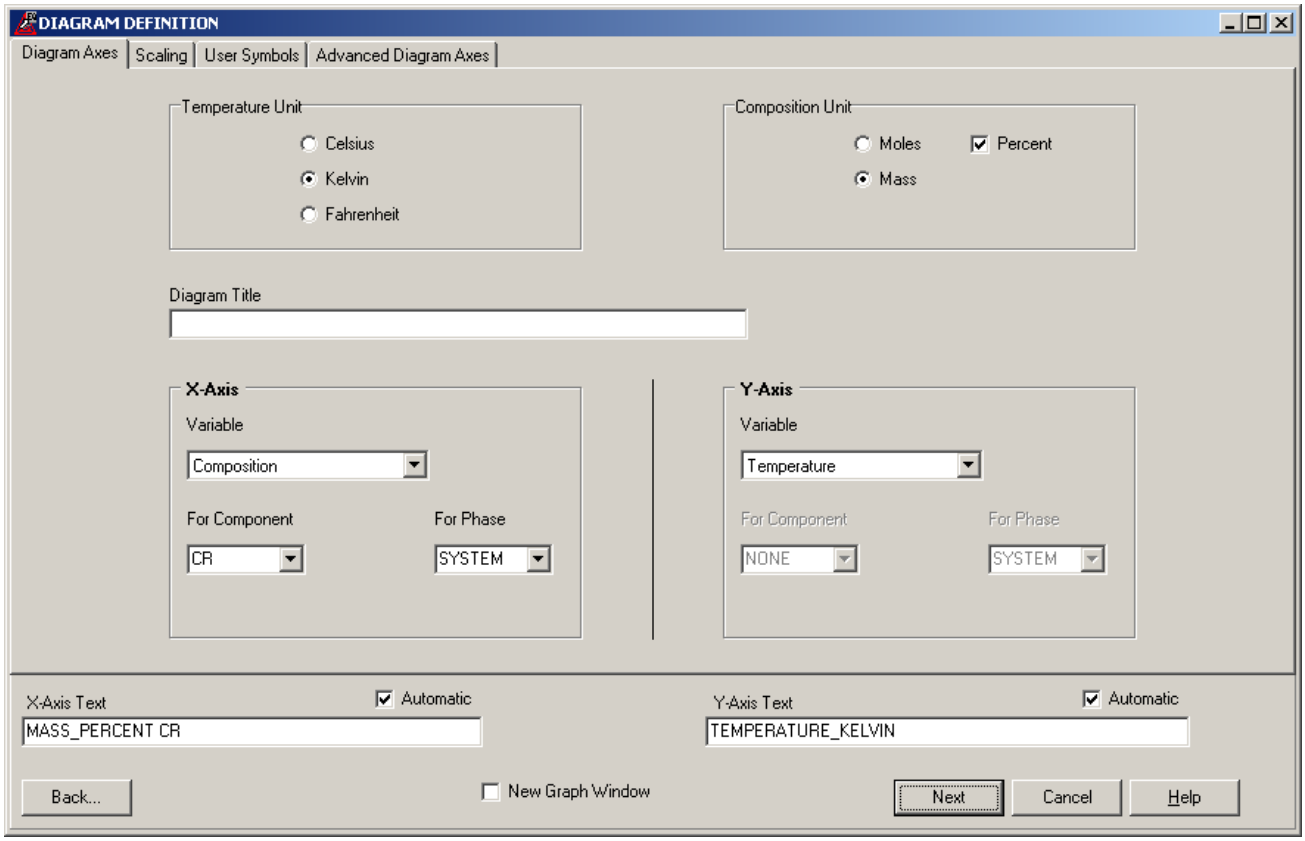
Functional Keys

Back	Got the CONDITION Window
Script Management	Open the Script window See 6.3.1
Next	Perform the Step or MAP calculation, this may take many minutes. While the calculation is progressing a window indicate what is done in the calculation. The “cancel” button will abort the calculation.
Cancel	Close window without remembering selection/changes
Help	Show the THERMO-CALC Help page regarding present window/tab
Arrow on right edge	Show the third axis.

Tick Boxes

Overwrite Previous Calculation	Select to overwrite previous calculation or not.
Generate Automatic Start Points	Check this box to automatically generate start points to find all lines in the diagram. If this is not checked, the initial set of conditions is used as a starting point. Used only with 2 axes.

6.5 DIAGRAM DEFINITION



In this window, a diagram from the MAP/STEP calculation can be defined.

Fields

X-axis Text	Show text plotted in the diagram near x-axis.
Y-axis Text	Show text plotted in the diagram near y-axis

Check box

Automatic	If checked the X-/Y-axis Text is set depending on the chosen plot axis property.
New Graph Window	If checked the new diagram is plotted in a new window.

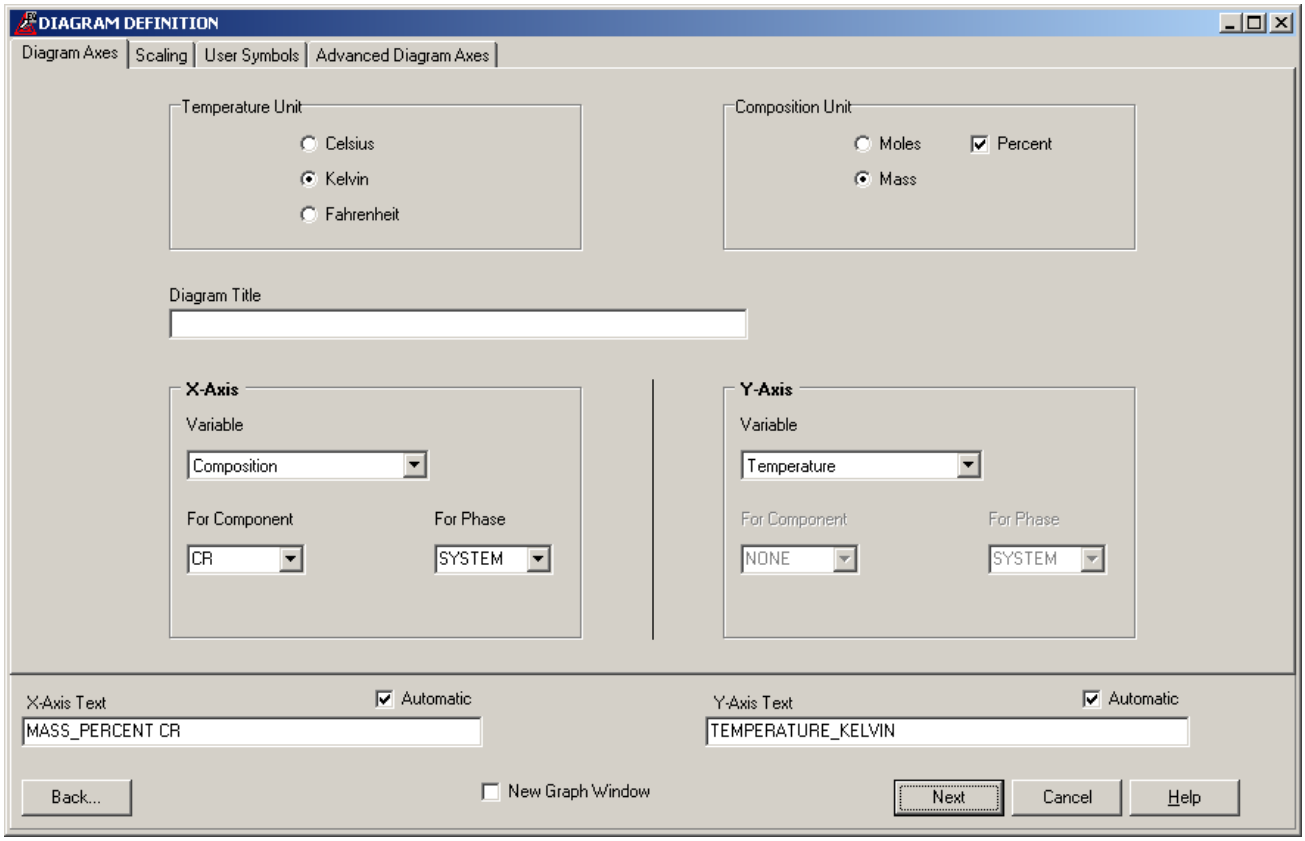
Functional TABS

Diagram Axes / Scaling / User Symbols / Advanced Diagram Axes — See section 6.5.1-4

Functional Keys

Back…	Go to MAP/STEP DEFINITION window
Next	Plot diagram and go to GRAPH window
Cancel	Close window without remembering selection/changes
Help	Show the THERMO-CALC Help page regarding present window/tab

6.5.1 TAB: Diagram Axes



Make settings for what to plot. Choose composition and temperature units. Optionally add a title for the diagram. Select from the fields what property to plot.

Both axes can plot the same variables and the instructions are the same.

Many more options for the selection of axis properties are available under the Advanced Diagram Axes tab.

Radio Button

temperature Unit	Set the unit to use if temperature is plotted
Composition Unit	Set the unit to use if composition is plotted

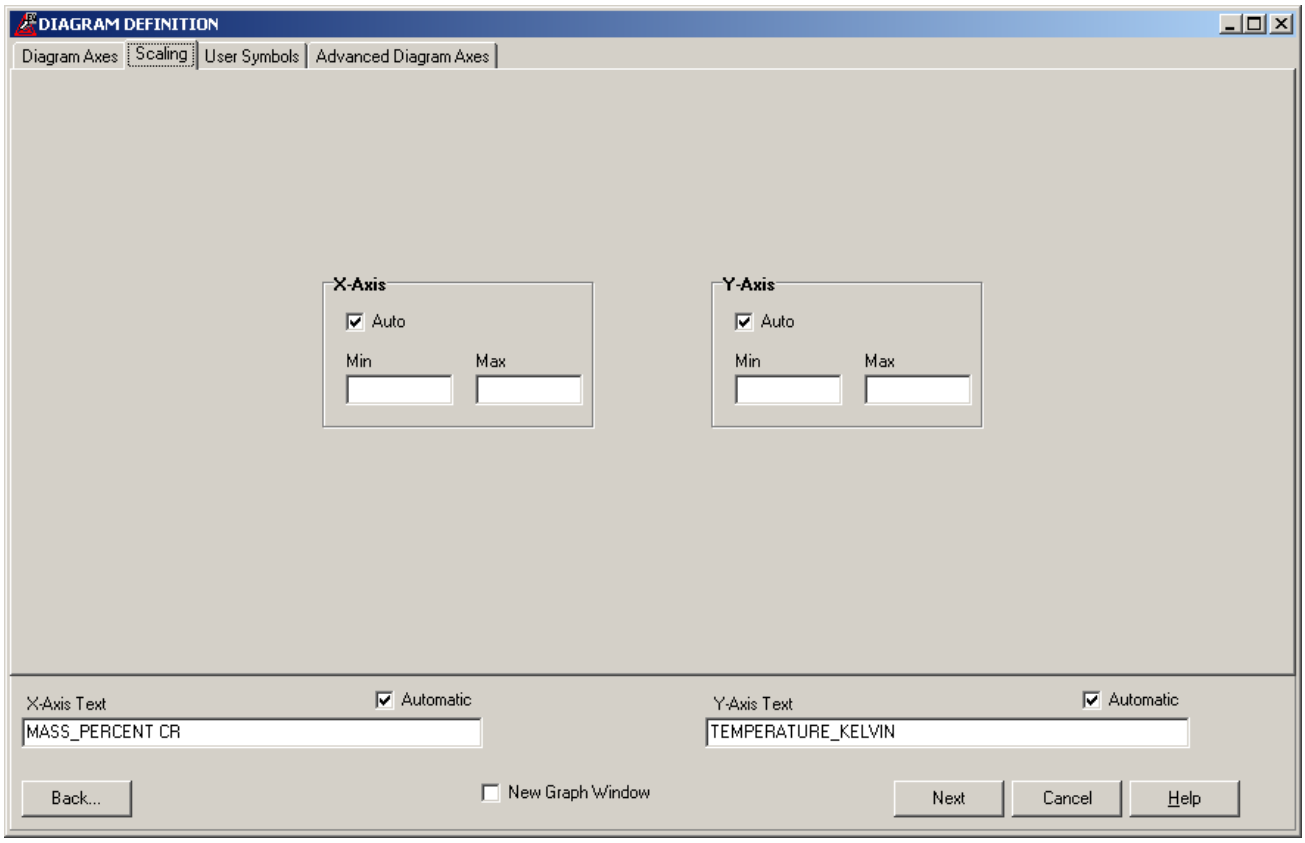
Fields

Diagram Title	If desired, give your diagram a title.
X- / Y-Variable	Chose what property to plot.
For Component	If needed specify property further.
For Phase	If needed specify property further.

Tick Boxes

Percent	If checked Mass- / Mole-Percent is plotted.

6.5.2 TAB: Scaling



The desired axis intervals for the plotted diagram can be controlled in this window.

If the Auto check box is checked, the axis interval is controlled automatically by the software.

To define other axis intervals, simply un-check the auto box and type in the desired axis intervals.

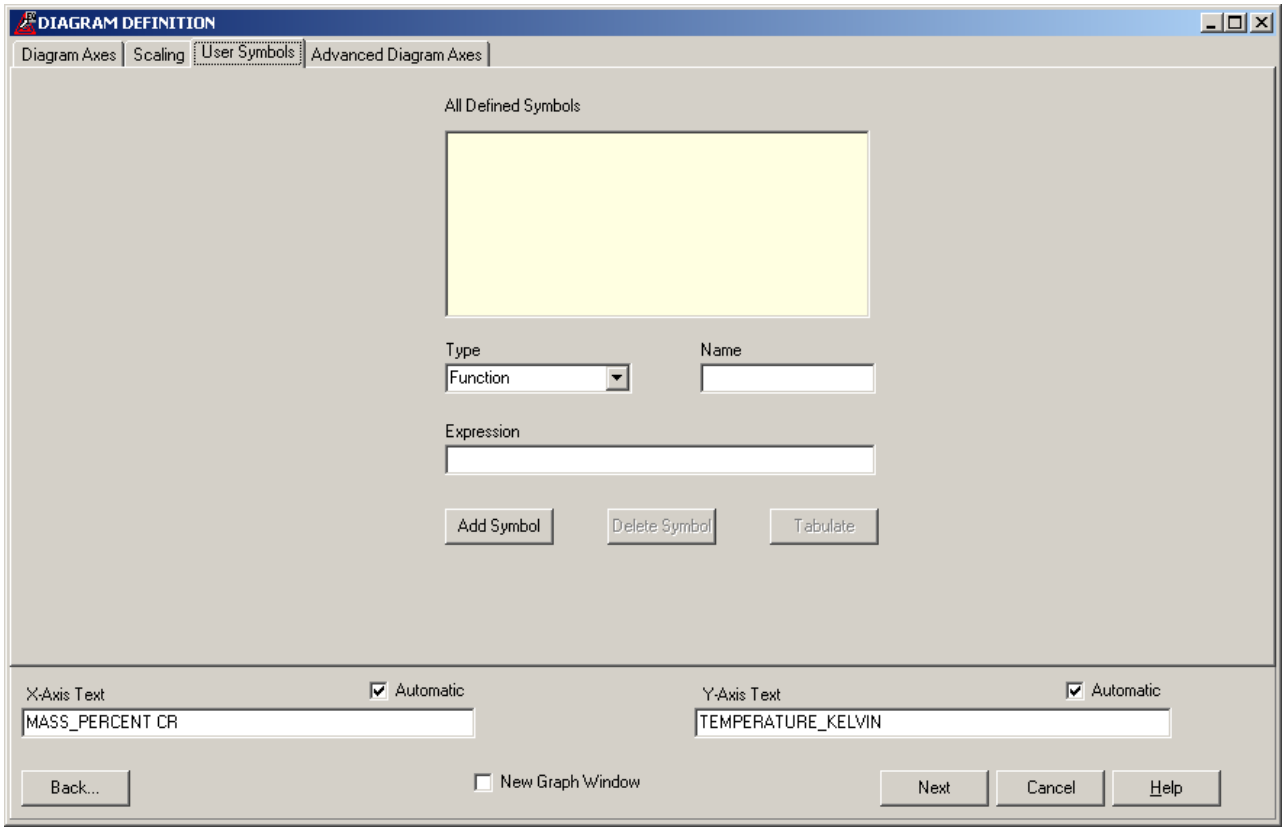
Fields

Min / Max — Choose the minimum and maximum limits to be plotted.

Tick Boxes

Auto — Uncheck the auto box to type in custom min and max values for the axis.

6.5.3 TAB: User Symbols



Under this tab the user may enter symbols to be plotted.
Type the expression for the symbol in the “Expression” field and give the symbol name in the “Name” filed then add it to the list by pressing the “Add Symbol” button. See also 6.3.2.

Fields

All Defined Symbols — Enter own symbols to be plotted. Here all the symbols already defined are displayed.
TOGGLE marked symbol by holding down *Ctrl* while clicking it in the list.
EDIT a symbol by marking it in the list, then edit the Expression, or Name field and press the “Add Symbol” button when done. Changing the “Type” field while doing an edit may delete the marked symbol.

Type — Constants: are just a means of using a name for a numeric value.

Functions: are expressions of state variables or other functions. These expressions are saved, and whenever a function value is requested all functions are evaluated.

Variables: are similar to functions because they can also be expressions of state variables. However, contrary to functions, they will only be evaluated when they are entered or if they are explicitly called upon.

Tables: are made by entering functions or variables defined in THERMO-CALC5 per default or previously entered by the user and separated by a space or a coma. The user symbols defined here can be seen also (and calculated and shown) in the THERMO-CALC CONDITIONS window under the User Symbols tab.

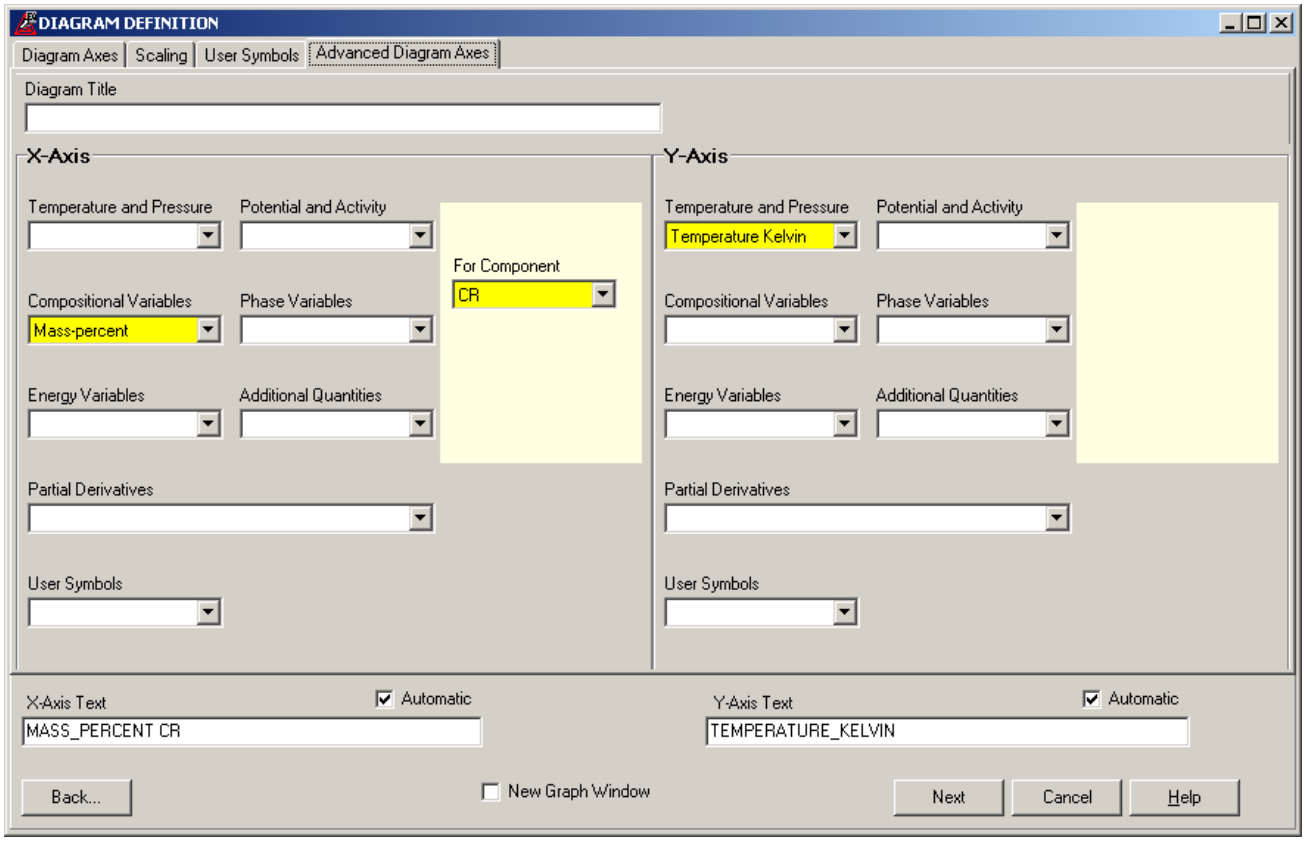
Name — Name for the symbol to be entered.

Expression	Enter a numeric value, or an expression of state variables or other functions.

Functional Keys

Add / Delete Symbol	Add / Delete the marked symbol defined in the symbols list.
Tabulate	After selecting a table symbol from the list. Pressing this button gives you the choice to write the calculated table to a window or a named file.

6.5.4 TAB: Advanced Diagram Axes



Fields

Diagram Title — If desired, give your diagram a title.

X- / Y-axis — From one of the combo boxes, select the property to plot on the axis.
Properties are sorted into eight combo boxes according to type.
If further distinction is possible related combo boxes appear in the rightmost column.

Tick Boxes

SER Reference State — If checked, the reference state is used.

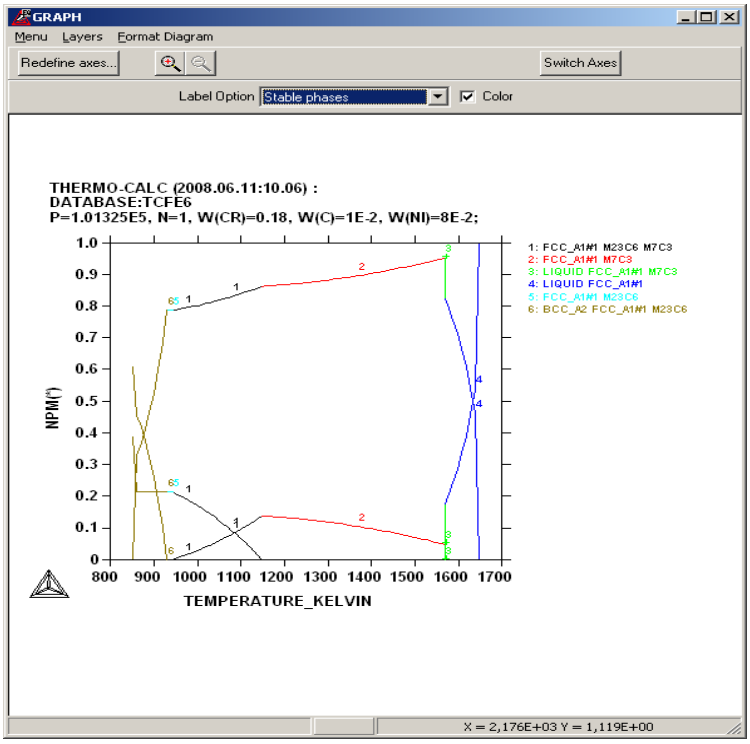
6.6 GRAPH

In the THERMO-CALC GRAPH window, plotted diagrams are displayed. The diagrams can be printed or saved as image files e.g. so they can be included in a written report. The final graphical property or phase diagram can be saved in the following graphical formats: Portable Network Graphics (.png), Windows Bitmaps (.bmp), Portable Document Format (.pdf), Joint Photographic Experts Group (JPEG) Format (.jpg), Tagged Image File Format (.tif), PostScript File (.ps), Microsoft Windows Enhanced Metafile (.emf) or Thermo-Calc's own experimental format (.exp) for later edit or inclusion/combination with other calculated diagrams.

A saved diagram can be opened in other programs for demonstration purposes. Only the Thermo-Calc experimental (.exp) file can be reopened in THERMO-CALC, all other formats are for use outside THERMO-CALC.
By saving the diagrams in the Enhanced Metafile (.emf) format the appearance of the diagram may easily be modified using external software.

NOTE: Please note that these functions require that the enclosed Ghostscript software is installed.
This is included on the installation CD.

6.6.1 Functions after Stepping



A property diagram can be saved in a format suitable for Microsoft Excel by using “Export to Excel” in the GRAPH-window Menu.
The coordinates of a plot can be saved to a text-file (.exp file) and .exp files with previously calculated plots can be appended for comparison.

Mouse Pointer Functions
Placing the pointer at a point of interest enables direct readings from the diagram. Coordinates are then displayed in the lower right corner of the window.
Placing the pointer in an area of interest and right click opens a Print or Save Diagram menu.
Placing the pointer on an Item (e.g. label) of interest and right click open Edit Item, Delete Selected Item, Print or Save Diagram.
Information about items identified by the pointer is displayed in the lower left corner of the window.

Menu bar

Menu	Print
	Save
	Export to Excel
	Append / Remove File(s), see 5.3.
Layers	Axis layer
	Legend layer
	Data layer
	Symbol layer
	Plotexp layer
	Top layer

Format Diagram	Tiangular Dagram Logarithmic X-axes Logarithmic Y-axes Display Conditions Raster Scaling Redefine Axis

Fields

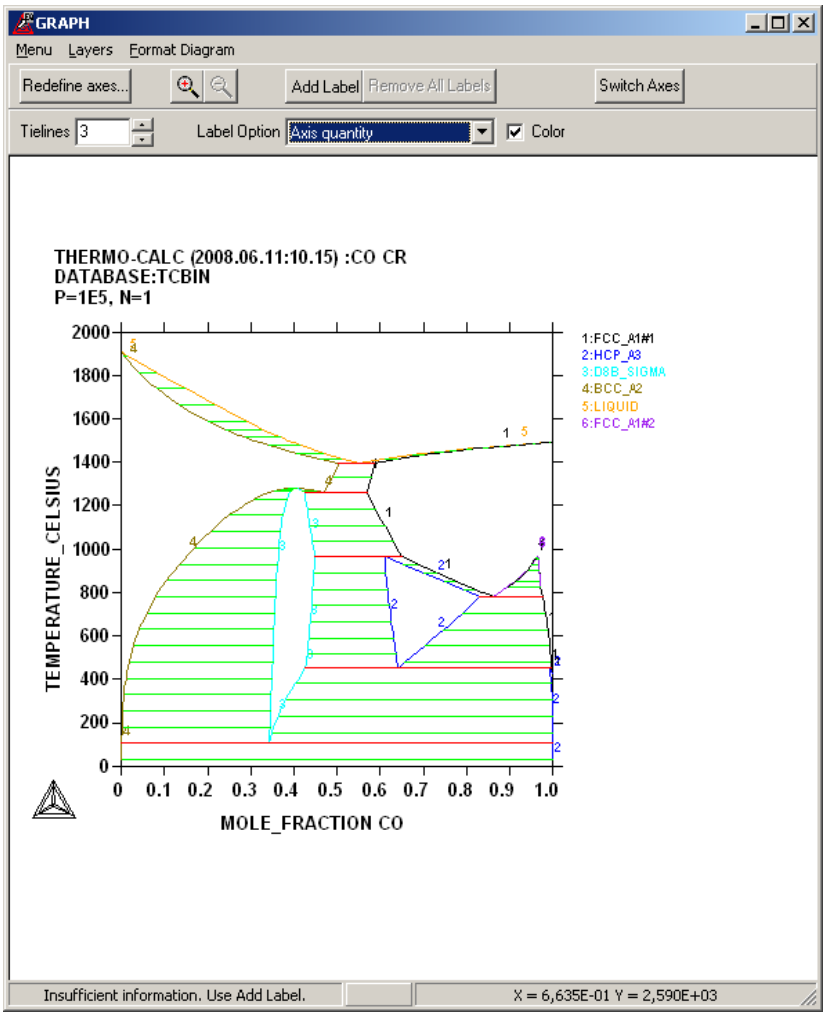
Label Options	Enter

Functional Keys

Redefine Axis	Choose Redefine Axes… from the Format Diagram menu or click the Redefine Axes… button on the THERMO-CALC GRAPH window to open the THERMO-CALC DIAGRAM DEFINITION window to change the diagram settings, for example the axis quantities and labels. This is useful for refining a plotted diagram or for defining a new diagram from the same MAPPING or STEPPING calculation.
Switch Axes	Click the Switch Axes button to switch the diagram axes (i.e. get the X variable on the Y-axes and the Y variable on the X-axes) without going back to the THERMO-CALC DIAGRAM DEFINITION window.
	Click the Zoom In (+) button to plot a small section of the diagram. Hold the left mouse button down and draw a rectangle section in the plot.
	Zoom out to the previous plot.

6.6.2 Functions after Mapping

All general functions are equal to what has been described in section 6.6.1.



Mouse Pointer Functions

Placing the pointer in an area of interest and right click open Add label, Print or Save Diagram.

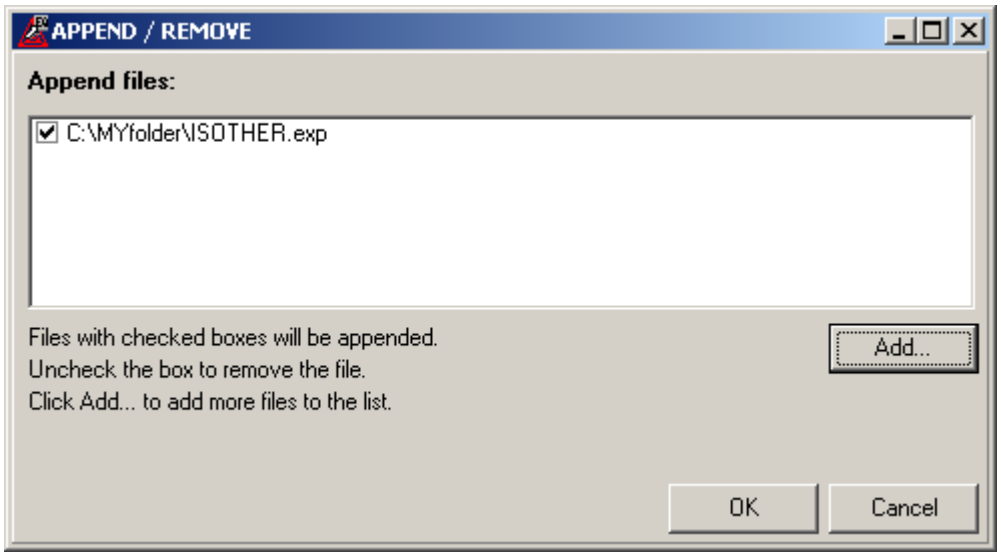
Placing the pointer on an Item (e.g. label) of interest and right click open Edit Item, Delete Selected Item, Print or Save Diagram.

Functional Keys

Add Label	If a phase diagram has been calculated and plotted on the THERMO-CALC GRAPH window, you may let the THERMO-CALC program to automatically write labeling texts that indicate stable phase assemblages on the plotted diagram.
Remove Label	Clicking the Remove Labels button will remove all the added labeling texts on the currently plotted phase diagram. To remove only one label, right-click on the selected label and choose Delete

6.6.3 Append File

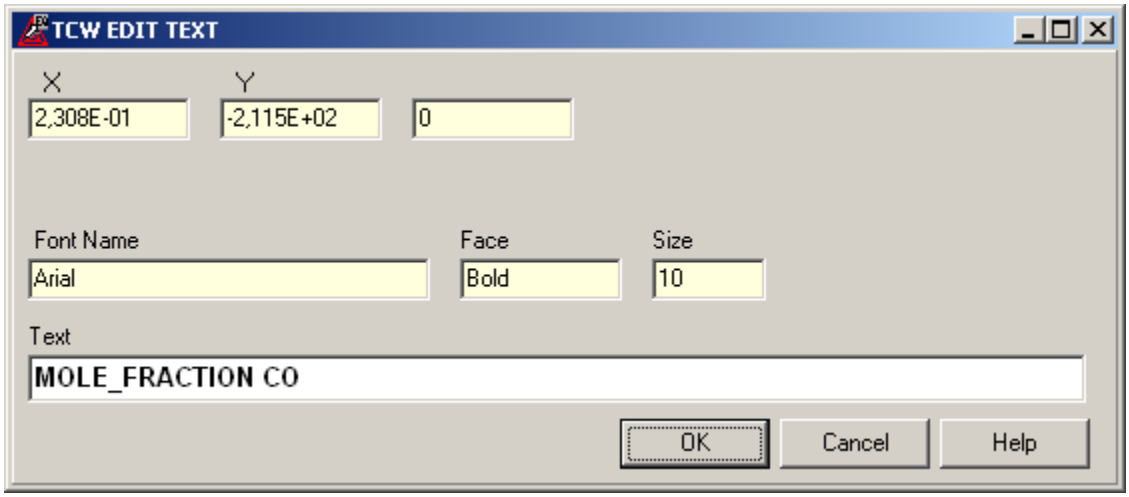
.exp files with previously calculated plots can be appended for comparison.



Click the “Add” key to add files to the Appended files list. An Open File dialog will be opened to let you choose one or more files.

6.6.4 Edit Text

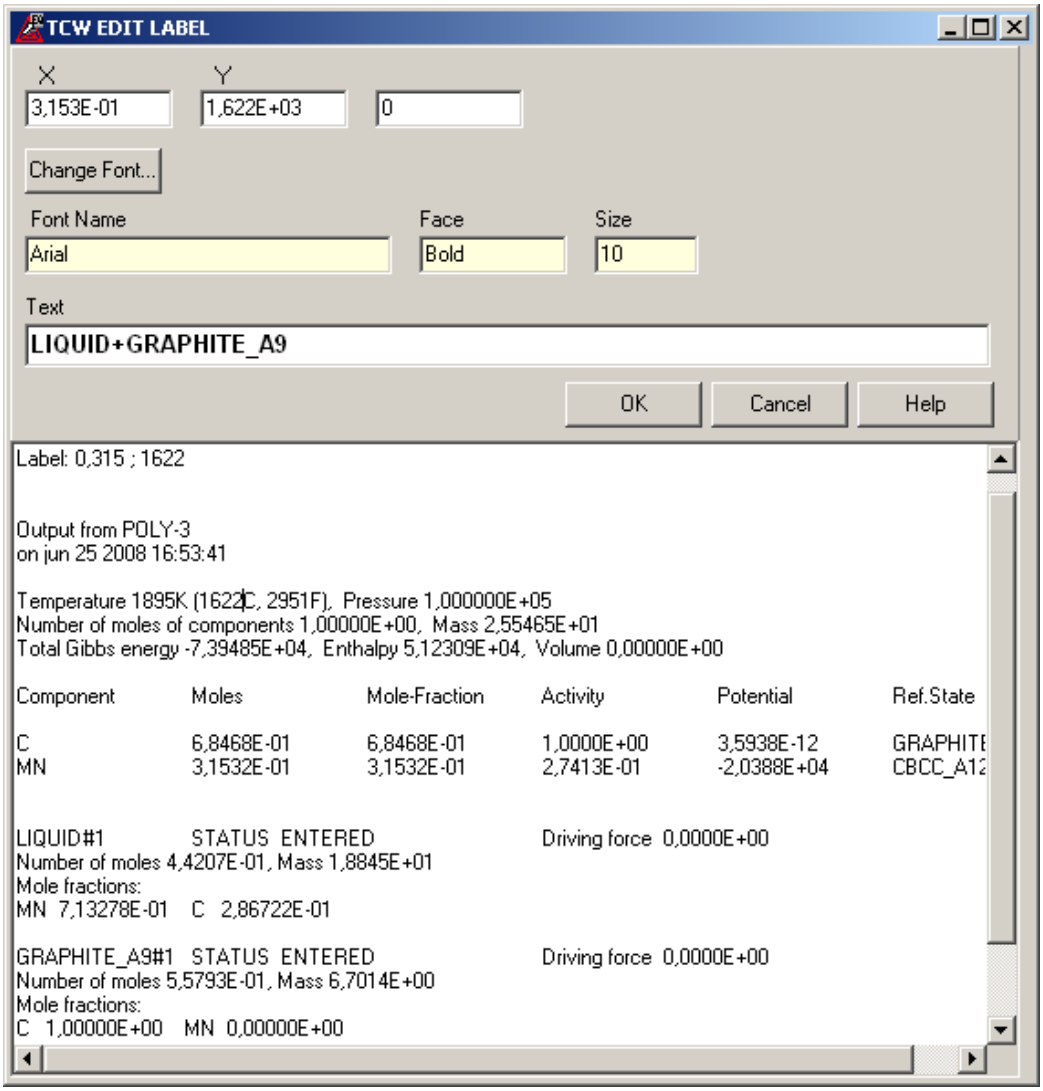
Place the mouse pointer on an axis text item and right click. Select “Edit Selected Item”.



6.6.5 Add label

To add llabel text fast, click the “Add Label” button. Until it is clicked again you may add labels to the diagram by left clicking in the data area of the graph window.

6.6.6 Edit Label



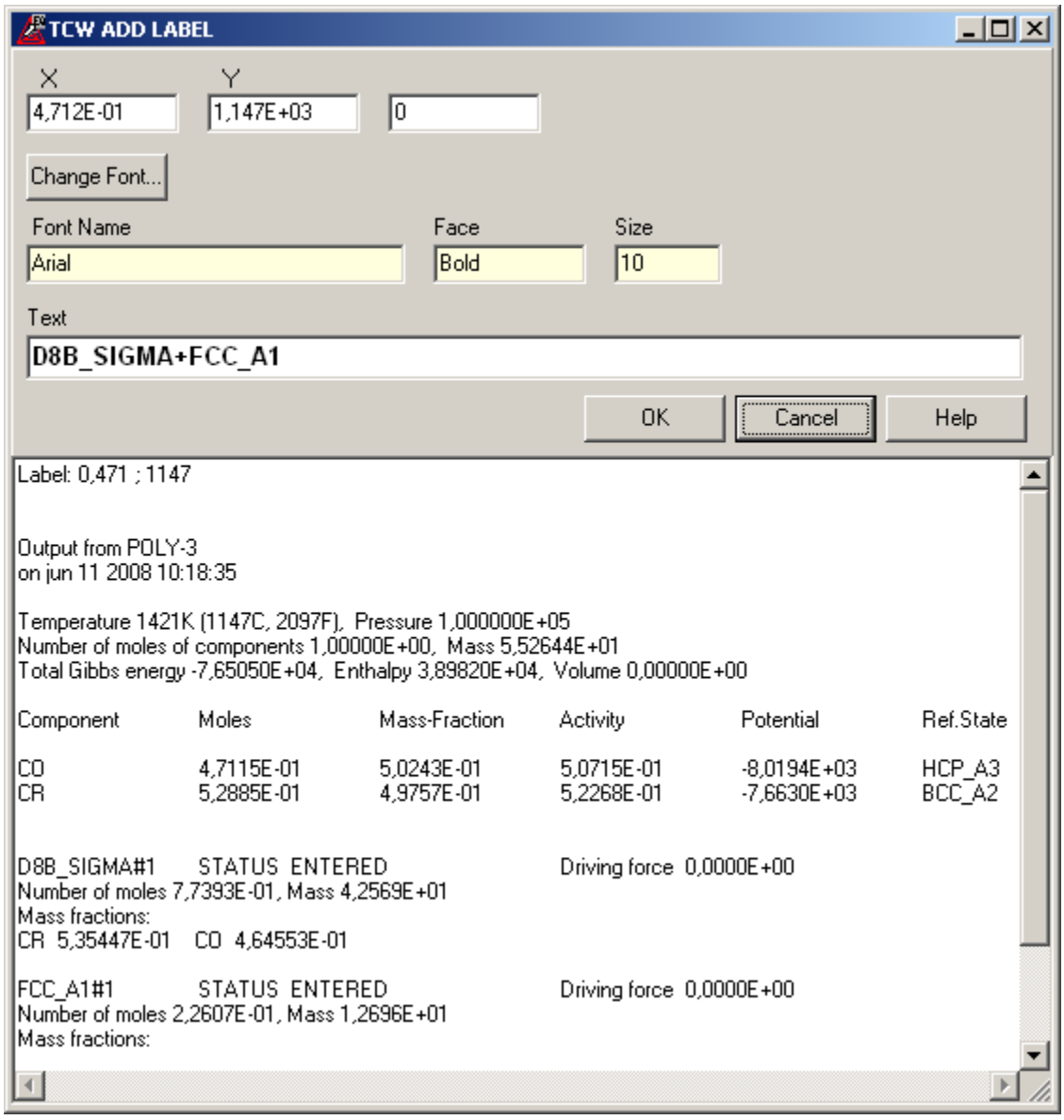
Place the mouse pointer on a label and right click. Select “Edit Selected Item”.

The program will automatically write the labeling text for that specific phase region on the plotted phase diagram, with the starting (left-most) X-/Y-coordinates for the assemblage texts being the position of the mouse. Repeat the above procedure for making other necessary labels for the phase regions on the entire phase diagram.

All such added labeling information will be used when the currently plotted diagram is zoomed, printed or saved.

6.6.7 Read Equilibrium Data From Plot

Place the mouse pointer in your diagram where you would like to perform your equilibrium calculation and right click. Select “Add Label…”



To add the label Text at the point where you made your calculation Click the OK button.

To copy the Equilibrium data, select the text by placing the pointer in the field, click and mark by moving the mouse. Place your pointer on the marked area, right click and select copy.

7 MAIN: MATERIALS MODULE

Click the Materials button in the THERMO-CALC Main window to start the Materials module. Different materials can be defined and stored on file in this module. This feature enables the user to define and name folders with materials and very quickly perform different types of advanced calculations. After selecting the material (e.g. a stainless steel) a series of different types of calculations may be chosen. Note that the appropriate thermodynamic database has to be installed and defined in order to make the calculations.

7.1 SELECT MATERIAL

After clicking the “Material” button the THERMO-CALC SELECT MATERIAL window different materials i.e. certain elements, phases and compositions can be stored in predefined or user defined folders.

By placing the mouse cursor on a specific material and right hand clicking, a menu appears. By choosing new or edit the THERMO-CALC Create Material window appears.

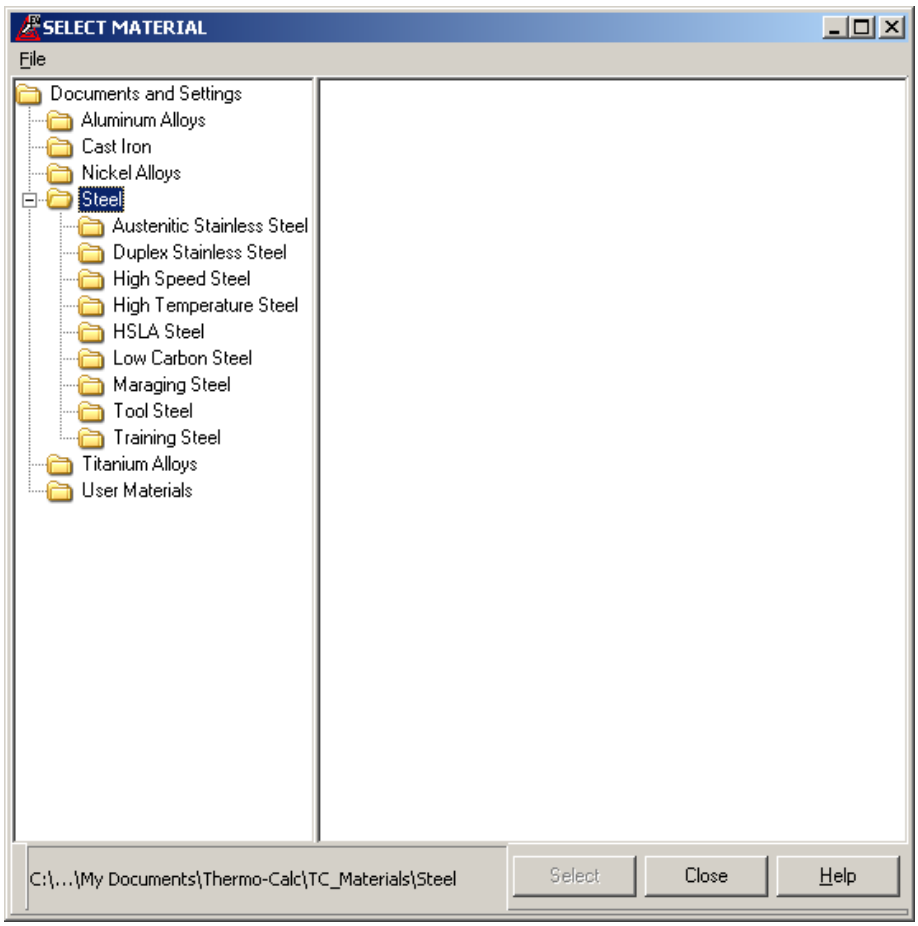
By clicking the Select Key a certain material is selected, and the THERMO-CALC Material Calculations window is opened.

Menu Bar

File — Enter a new material, Create Material, or edit an existing material.

Functional Keys

Select — Start the Material Calculations.



7.2 CREATE MATERIAL

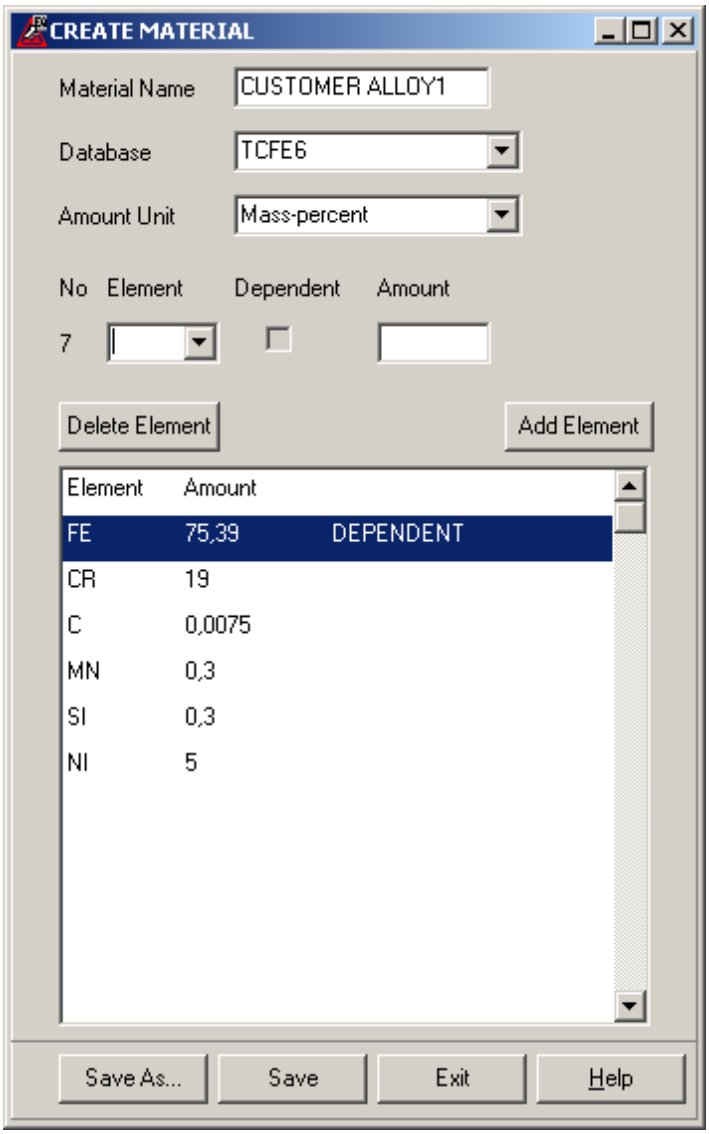
The THERMO-CALC Create Material window is opened by File/New in the menu in the Select Material window, or by placing the mouse cursor on a specific material, right hand clicking the mouse and choosing edit new.

Specify the Material Name.

Select the database to be used in the calculations. Note that in case a database is upgraded to a newer version, you must also update the material(s) by edit or the predefined material will keep using the database version as specified when the material was created.

Select the components, given by the database, and specify the dependant component and give the composition.

Note that the composition can temporarily be changed during the calculations when using the material in the materials module. The composition can later be changed by editing the material.



7.3 MATERIALS CALCULATIONS

7.3.1 TAB: Material

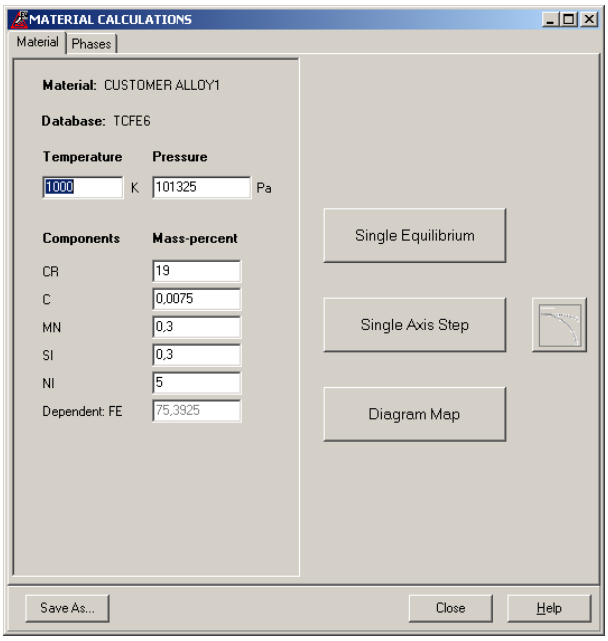
In the THERMO-CALC Material Calculations window different type of calculations may be set up.

First the temperature and the pressure should be defined, Thermo-Calc give proposals.

The composition of the material may be modified.

Then one of the following four types of calculations may be chosen:

- Single Equilibrium calculation
- Single Axis Step
- Diagram map.
- Scheil simulation

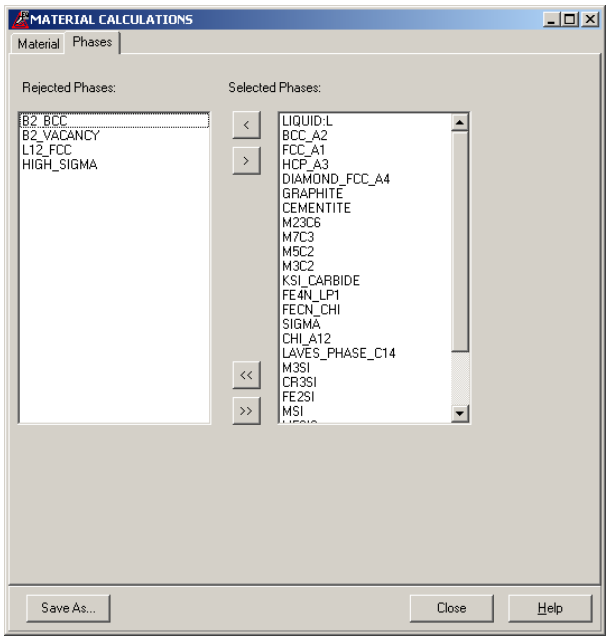


Functional Keys

Single Equilibrium	Perform single equilibrium calculations.
Single Axis Step	Step in one axis for e.g. calculating property diagrams.
Diagram Map	Map a diagram for the selected material.
Scheil Simulation	Scheil calculation solidification is simulated for the selected material.

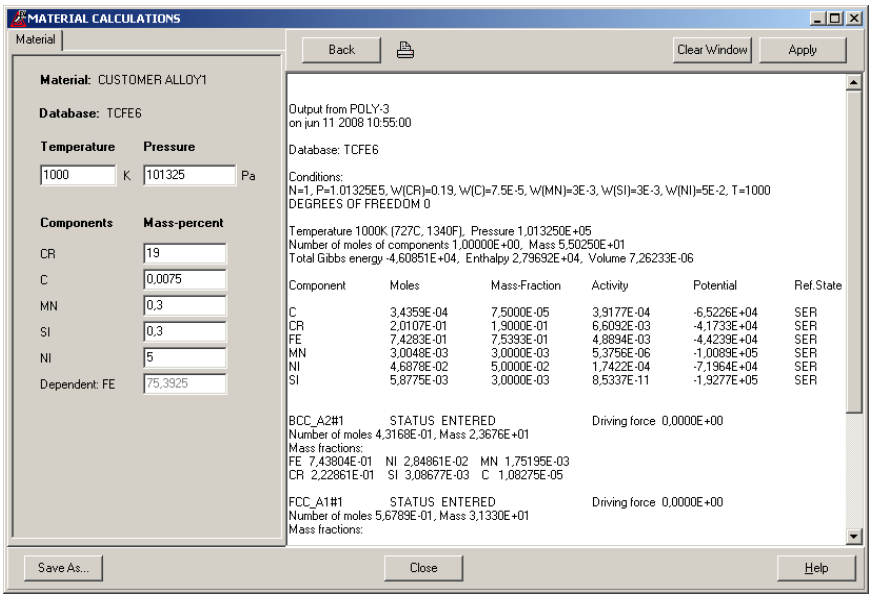
7.3.2 TAB: Phases

Here the phases to be included or rejected in the calculation may be specified.



7.3.3 KEY: Single Equilibrium

Here a single equilibrium for different set of conditions may be calculated.
It is also possible to modify the composition or conditions of the material to study how the composition will influence e.g. the equilibrium fraction of phases.



Functional Keys

Back	go to before single equilibria
Printer	print equilibria data
Clear window	clear window where equilibria data is shown
Apply	Click here to perform a new equilibrium calculation, possibly with different conditions

7.3.4 KEY: Single Axis Step

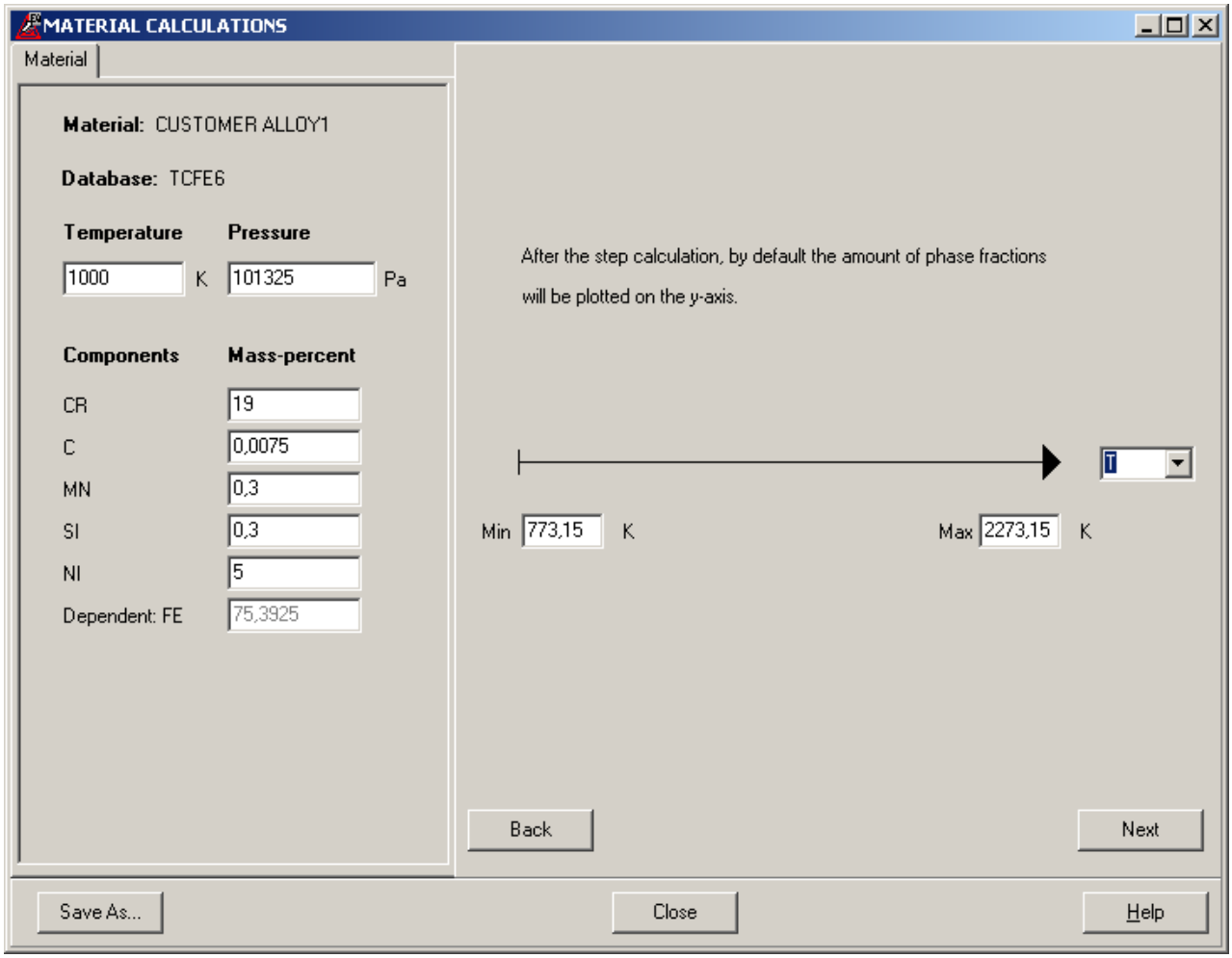
Here a stepping calculation along one axis may be performed.

To the left the conditions are specified, which can be modified.

The right hand side of the window shows the variable to be varied during the stepping.
T for temperature has been selected below.

Also specify its min and max values.

By clicking next the diagram is mapped and the result is plotted in the THERMO-CALC Graph window.



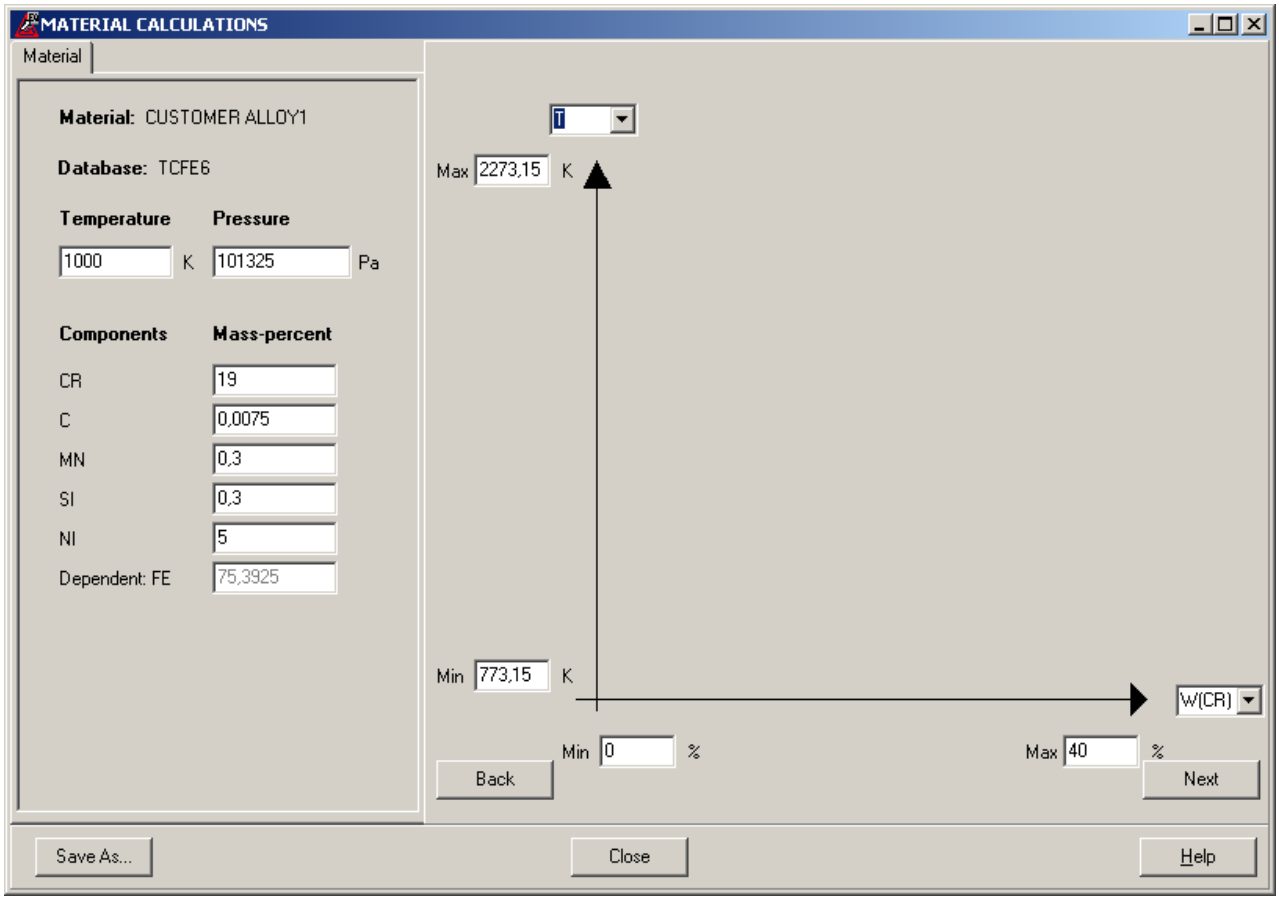
7.3.5 KEY: Diagram Map

Here a diagram may be mapped.

To the left the conditions are specified, which can be modified.

The variables on the two axes should be specified, including the min and max limits.

By clicking Next the diagram is mapped and the result is plotted in the THERMO-CALC Graph window, see 1.6.

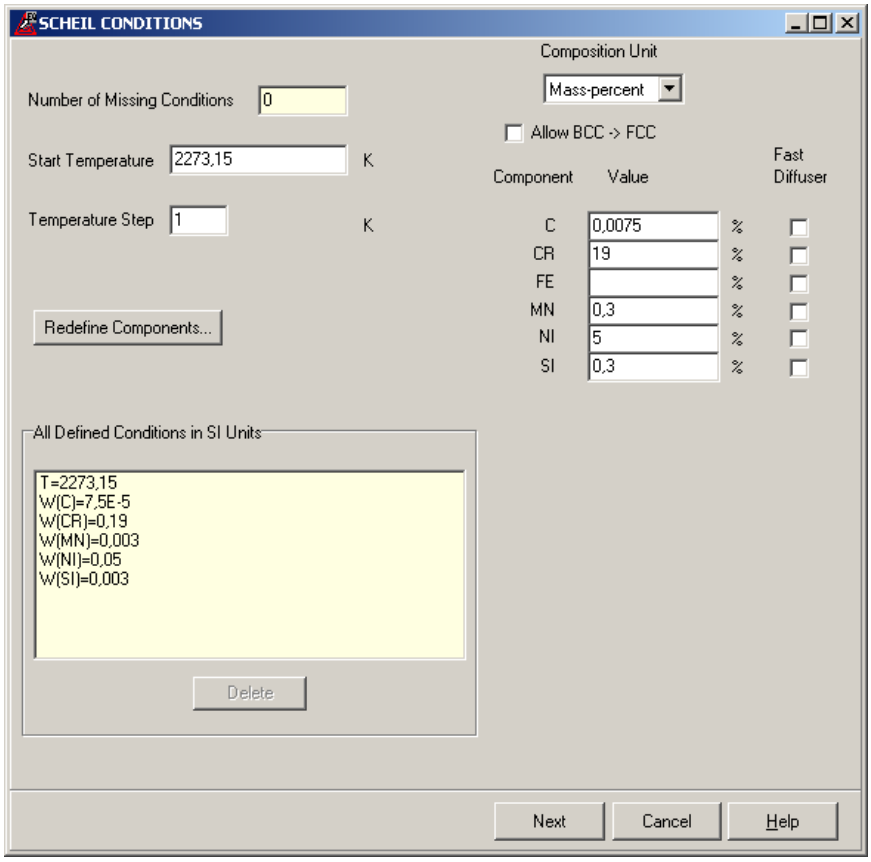


7.3.6 KEY: Scheil Simulation

In the THERMO-CALC Scheil Conditions window a Scheil calculation for the specified material is set up.

The conditions and composition are specified, which also can be modified.

By clicking “Next” the calculation is performed and the result is plotted in the THERMO-CALC Graph window.



Fields

Number of missing conditions	updated by clicking a field
Start Temperature	Enter start temperature for Sheil Simulation
Temperature Step	Enter temperature difference between consecutive equilibria in the simulation
Composition Unit	Choose composition unit for condition

Check box

Allow BCC -> FCC	Allow BCC phase to transform in to FCC phase when it is more stable
Fast Diffuser	Component is treated as a fast diffuser, increase computational time.

Functional Keys

Delete	Delete marked condition
Redifine Components	By clicking here the components may be redefined.

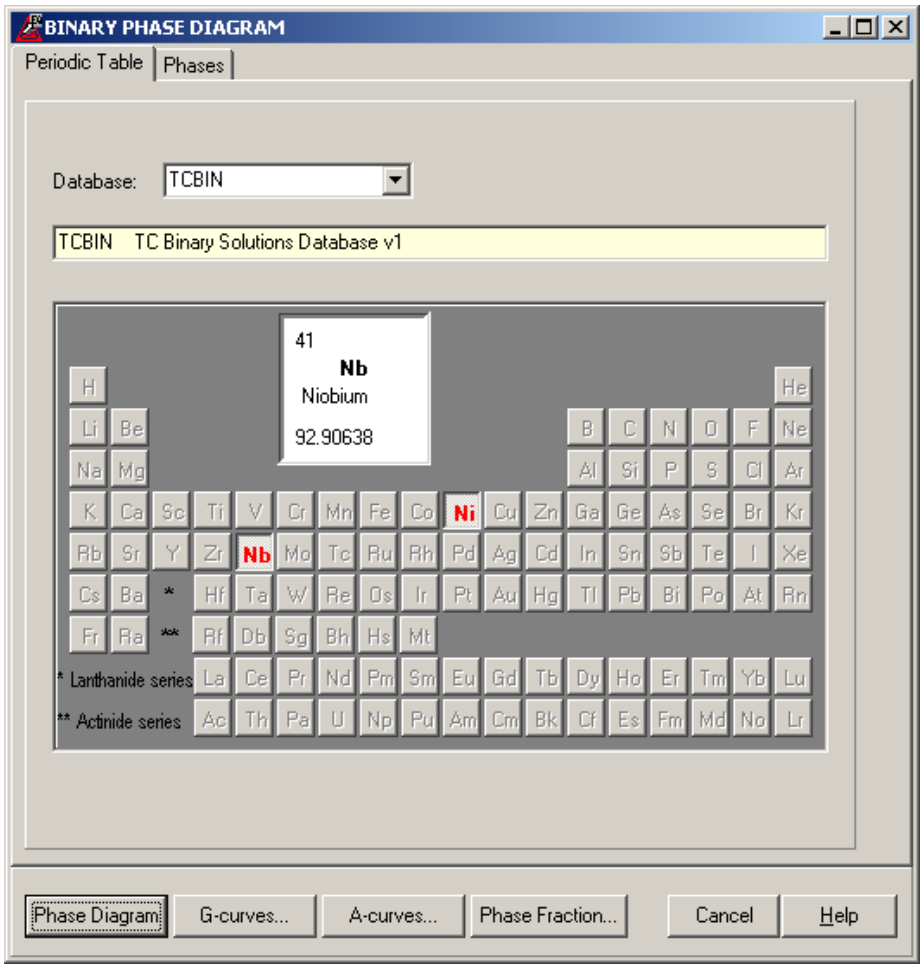
8 MAIN: TOOLBAR QUICK KEYS

8.1 BINARY PHASE DIAGRAM

Press the  key to the right on the toolbar in the Main window to start the Binary Phase Diagram Module. This is the specialized binary phase diagram calculation module. Here, the user can quickly calculate a binary phase diagram, the Gibbs energy curves, the activity curves, or the phase fraction for a binary system. Pressing this button open the periodic table containing the elements of the best binary database available.

8.1.1 TAB: Periodic Table

Select two elements.
The gray elements are not included within the database and cannot be chosen.
All of the elements turn gray when two elements have been chosen.



Functional Keys
Phase Diagram calculate the binary phase diagram

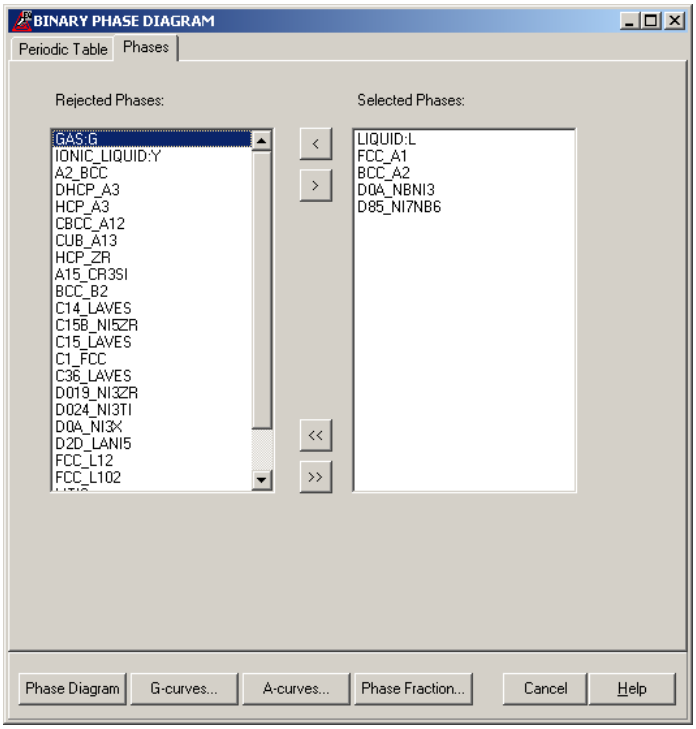
G-Curves	the Gibbs energy curves of each phase
A-Caruves	the Activity curves of each element
Phase Fraction	or the fraction of phases at a given composition.

8.1.2 TAB: Phases

In this window it's possible to specify the phases that the calculation will be based upon by rejecting undesired phases.
The phases appear only when the element(s) have been selected.

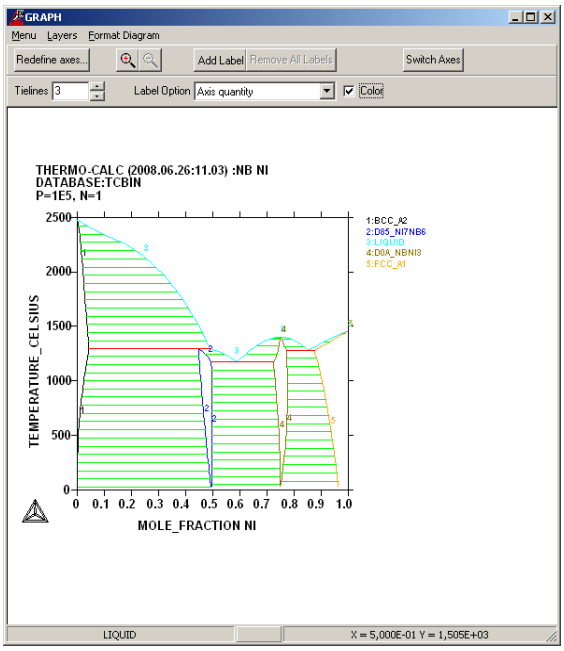
Functional Keys

Phase Diagram calculate the binary phase diagram
G-Curves the Gibbs energy curves of each phase
A-Caruves the Activity curves of each element
Phase Fraction or the fraction of phases at a given composition.



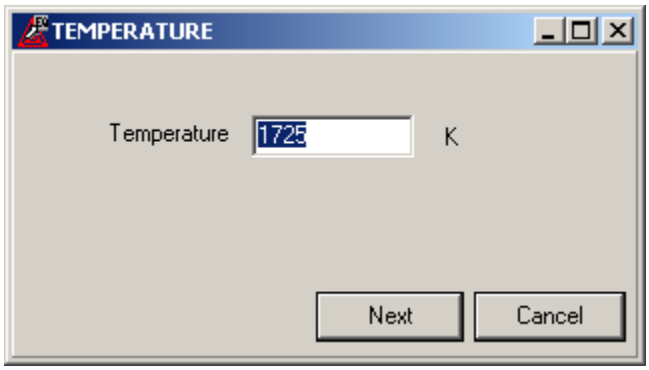
8.1.3 KEY: Phase Diagram

Select Phase Diagram and the diagram will appear in the Graph window.

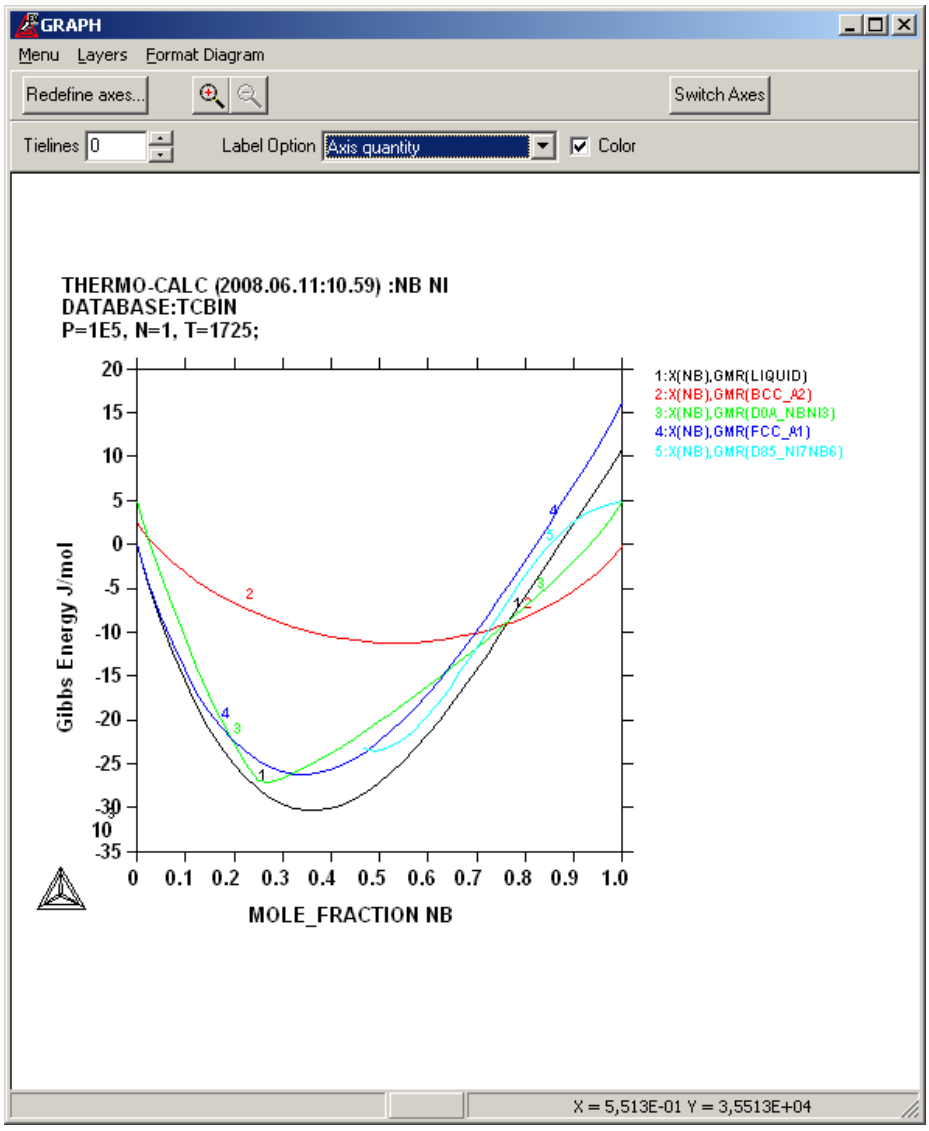


8.1.4 KEY: G-Curves

Select a temperature for calculating the (Gibbs free energy) G-Curves.

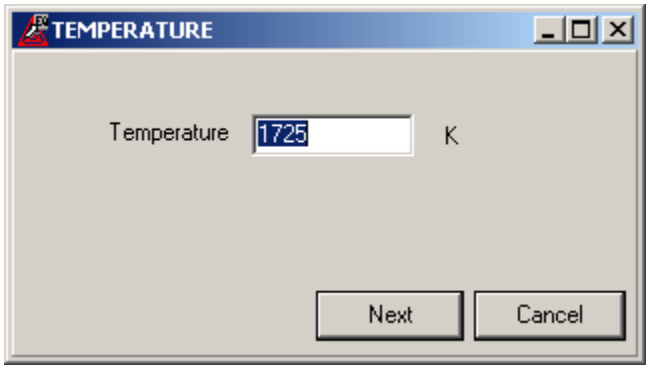


Pressing “Next” the diagram will appear in the Graph window.

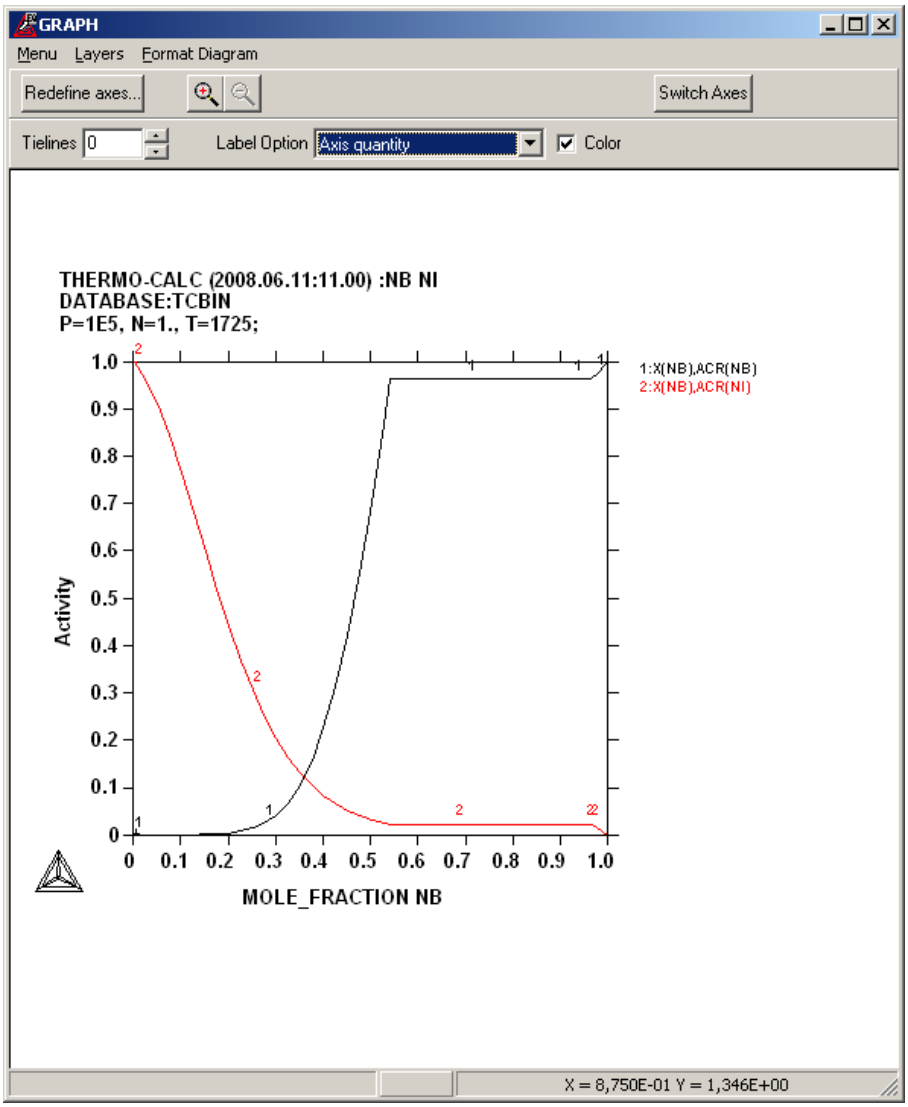


8.1.5 KEY: A-Curves

Select a temperature for calculating the G-Curves.

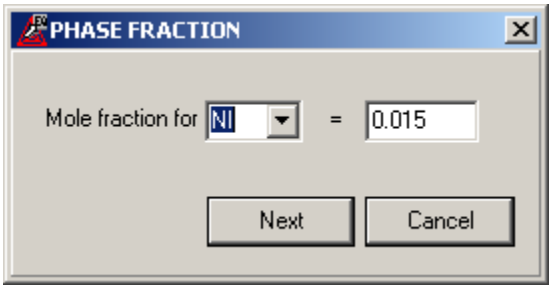


The diagram will appear in the Graph window.

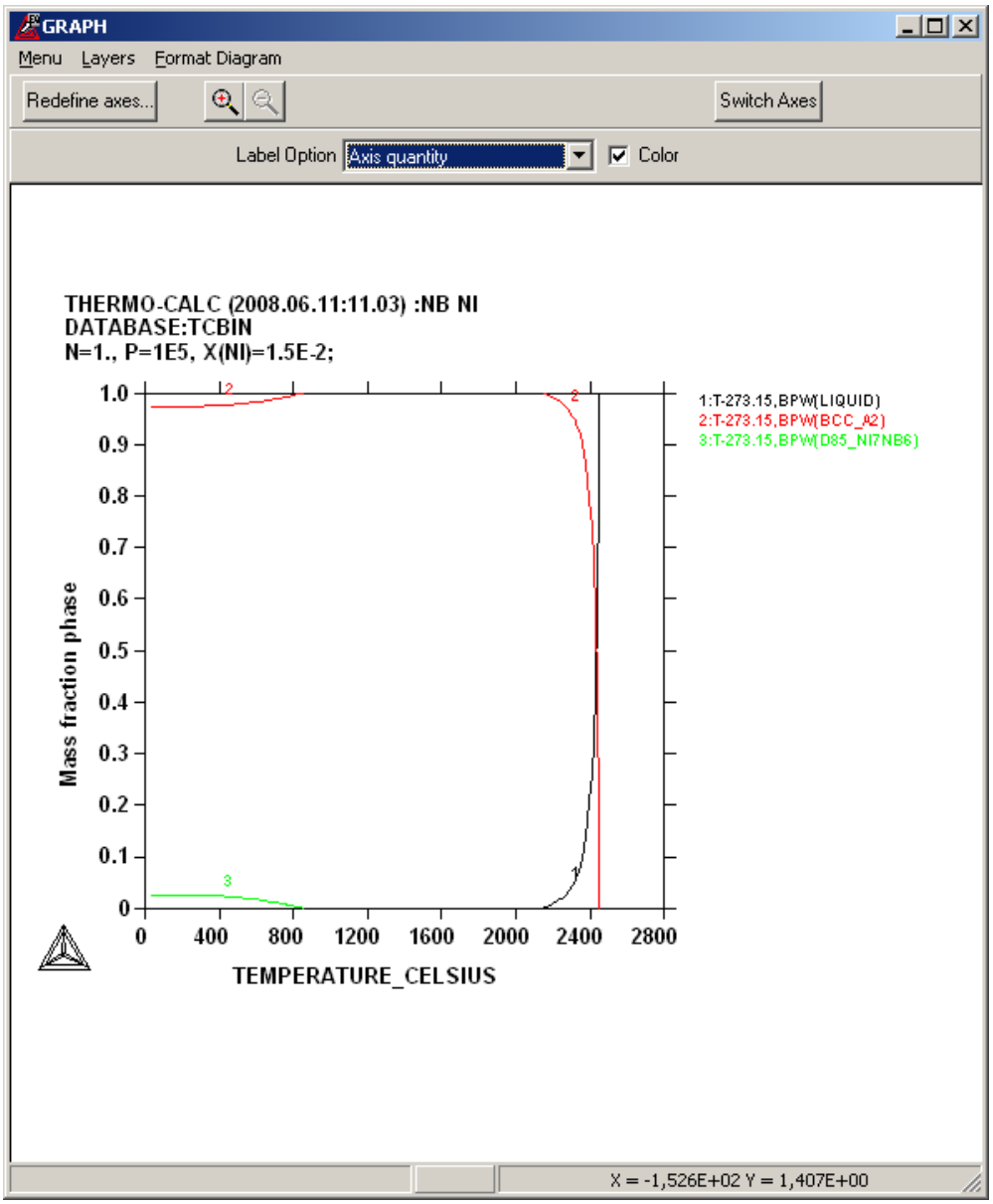


8.1.6 KEY: Phase Fraction

The stable equilibrium will be calculated at the given composition.
It is possible to choose the element for which the mole fraction is entered.



The diagram will appear in the Graph window, see section 1.6.



8.2 TERNARY PHASE DIAGRAM

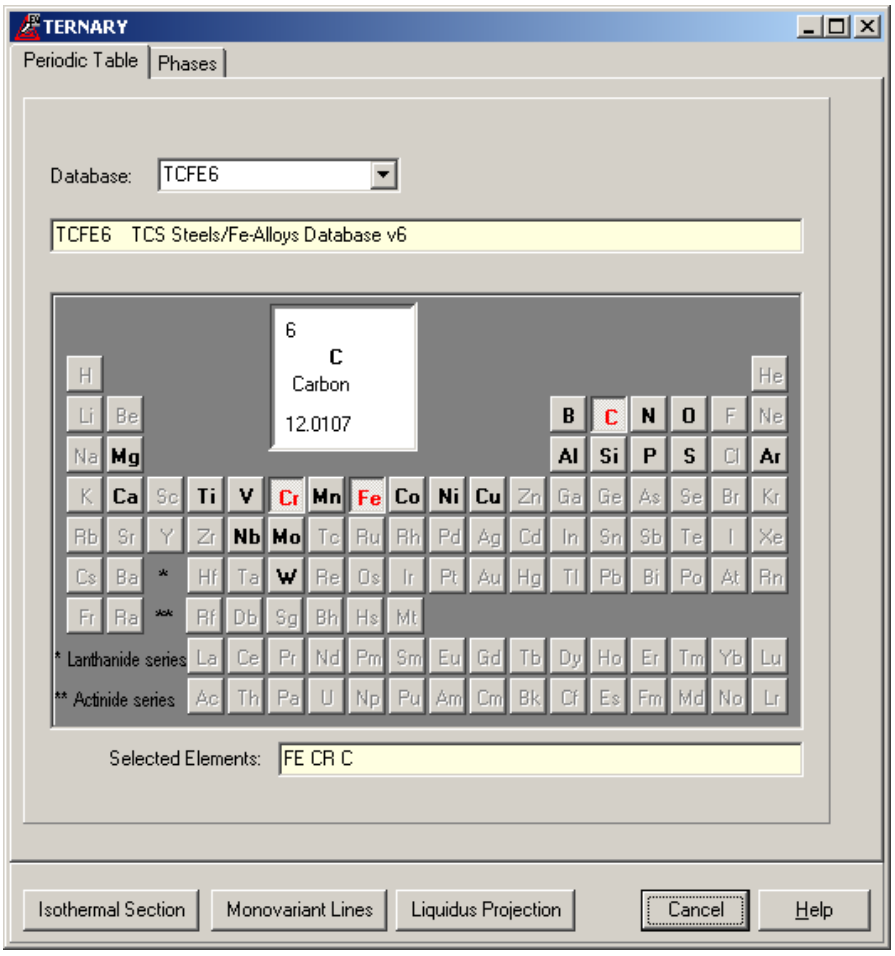
Press the key to the right on the toolbar in the Main window to start the Ternary Phase Diagram Module. In this module the user quickly and easily can calculate isothermal sections or liquidus projections in ternary phase diagrams.

The Ternary module enables quick calculations of:
Isothermal sections,
Projections of liquidus surfaces
Monovariant lines.

8.2.1 TAB: Periodic Table

Pressing this key starts the periodic table, where selection of the system is made and the type of calculation is chosen. In this window the available elements within the chosen database are displayed.

Choose the three particular elements by clicking on them, they turn read when selected.

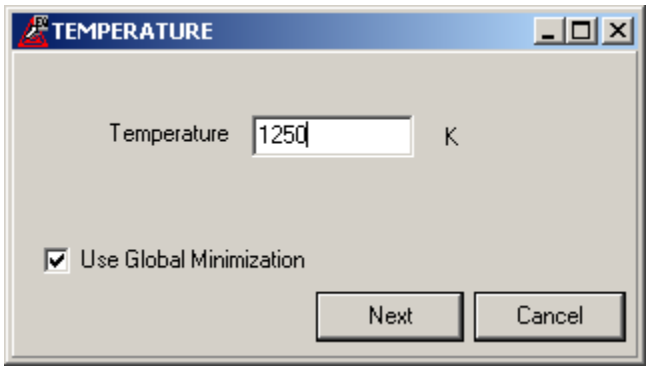


Functional Keys

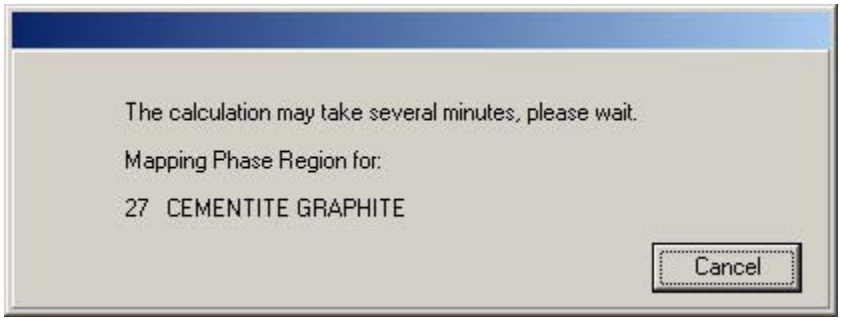
Isothermal Section	Enable calculations of isothermal sections
Monovariant Lines	Calculate the monovariant lines
Logarithmic Projection	Calculate liquidus projections

8.2.2 KEY: Isothermal Section

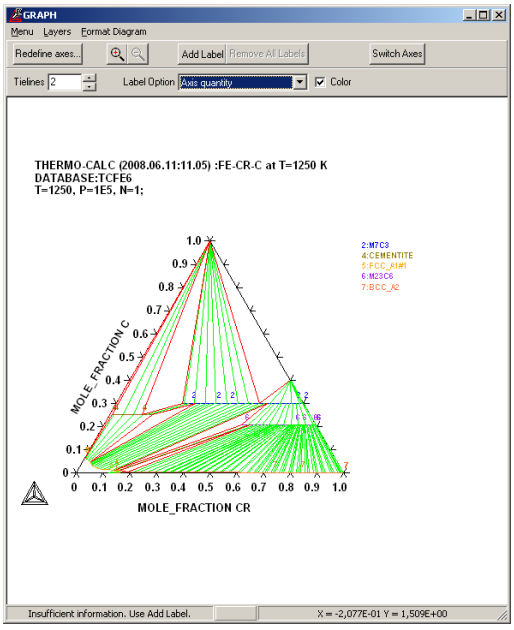
Here isothermal sections of ternary phase diagrams can be calculated. After defining the ternary system, specify the temperature in the Temperature Window.



Pressing Next start the calculation and show the window below. Pressing Cancel returns to the previous window. (Un)Checking “Use Global Minimization” box affects only the calculation at hand.

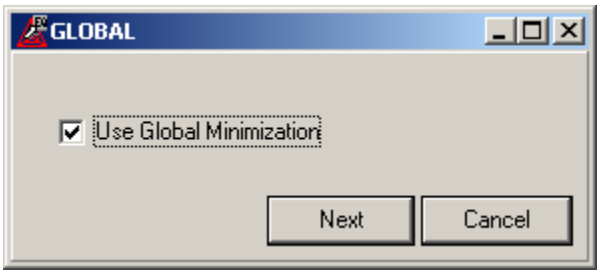


While the calculation proceeds a window will indicate what region in the diagram is calculated. Pressing Cancel returns to the previous window after finishing the present region. The diagram will appear in the Graph window.

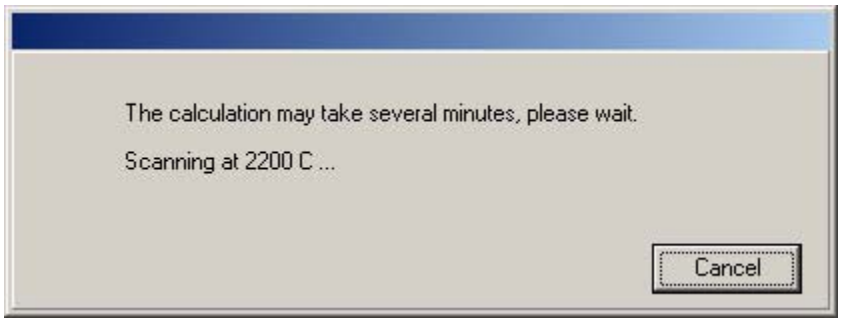


8.2.3 KEY: Monovariant Lines

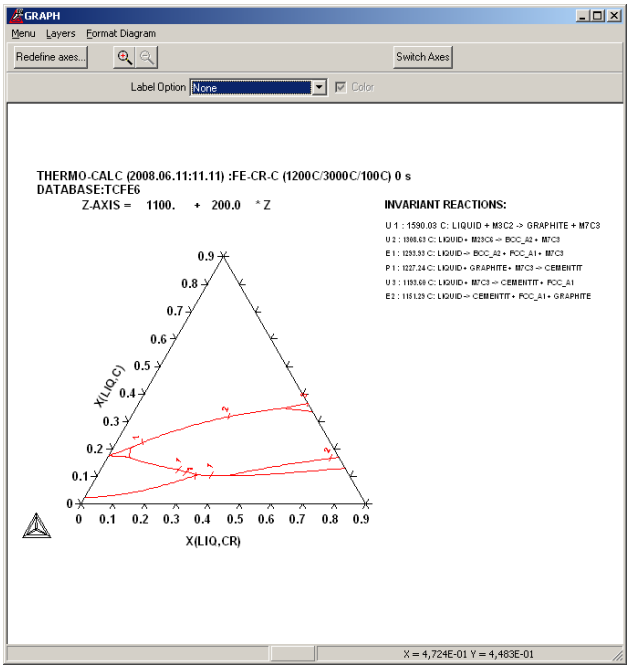
Set up the ternary system and then *click* the key for Monovariant Lines to calculate the monovariant lines in a ternary phase diagram. The diagram will appear in the Graph window.



(Un)Checking “Use Global Minimization” box affects only the calculation at hand. Pressing Next start the calculation and show the window below. Pressing Cancel returns to the previous window

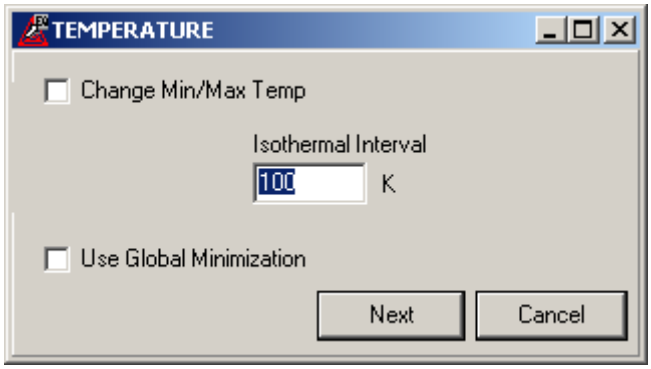


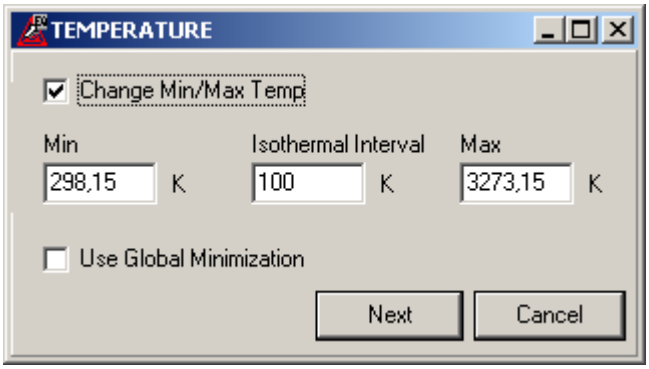
Pressing Cancel while the calculation is in progress aborts the calculation and returns to the previous window When the calculation is done the ersult is shown in the GRAPH window.



8.2.4 KEY: Liquidus Projection

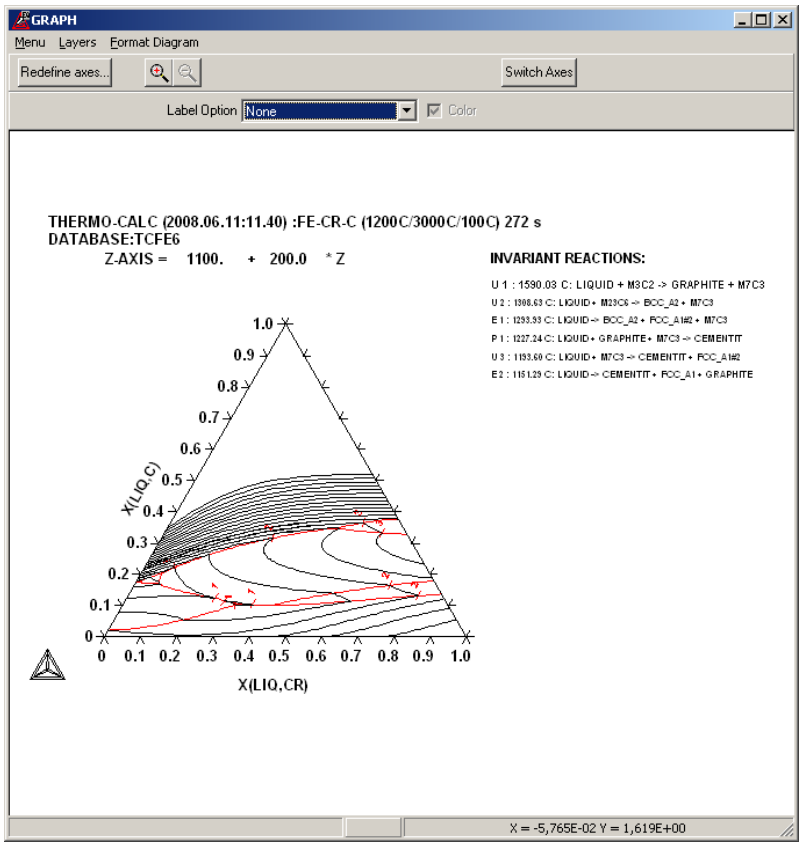
Click on the Liquidus Projection key to plot a projection of the liquidus surface
When starting a liquidus projection calculation a dialog box appears. In this box the temperature calculation interval can be specified. By pressing the next button the calculation is performed and the THERMO-CALC GRAPH window is opened when it is finished





Checkbox

Change Min/Max Temp	Enables the user to specify the min and max temperature.
Use Global Minimization	Unchecking / Checking affects only the calculation at hand.



8.2.5 TABs

Periodic Table and Phases, see 8.1.2

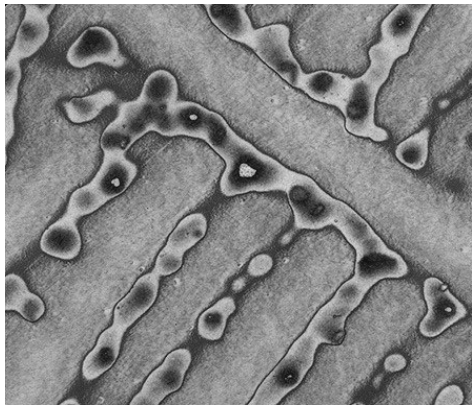
8.3 SCHEIL

Click the  key to the right on the toolbar in the Main window to start the Scheil Simulation Module. Here, the user quickly can simulate the solidification and micro segregation of an alloy using the Scheil-Gulliver model. This model assumes full equilibria in the liquid state and of no diffusion in the solid state.

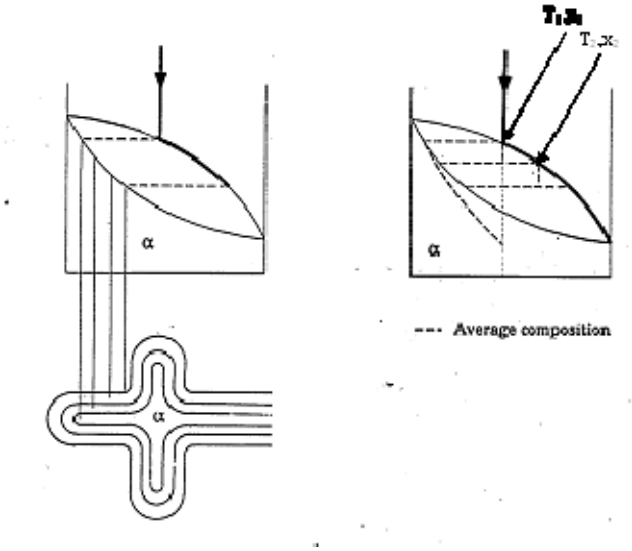
8.3.1 Theorethical Background

In order to account for microsegregation during solidification, a Scheil module has been implemented in Thermo-Calc for Windows.

In the Scheil-Gulliver model it is assumed that diffusion in the liquid phase is infinitely fast.
In the solid phases there is no diffusion i.e. no back diffusion.
Along each step in the cooling process, local equilibria establish at the solidification interface where the composition of the alloy may be significantly different from the overall composition, and the compositions of liquid and solid at the interface are given by the system's phase diagram. The solid phase formed will retain its composition from when it was formed whereas the liquid composition is always homogeneous. The Scheil-Gulliver model implemented in the Thermo-Calc for Windows software can be applied to any high-order multicomponent system. A simulation is made step by step along the cooling procedure, and after each step the new liquid composition is used as the “local overall” composition at the next step.



Microsegregations in cast microstructure.



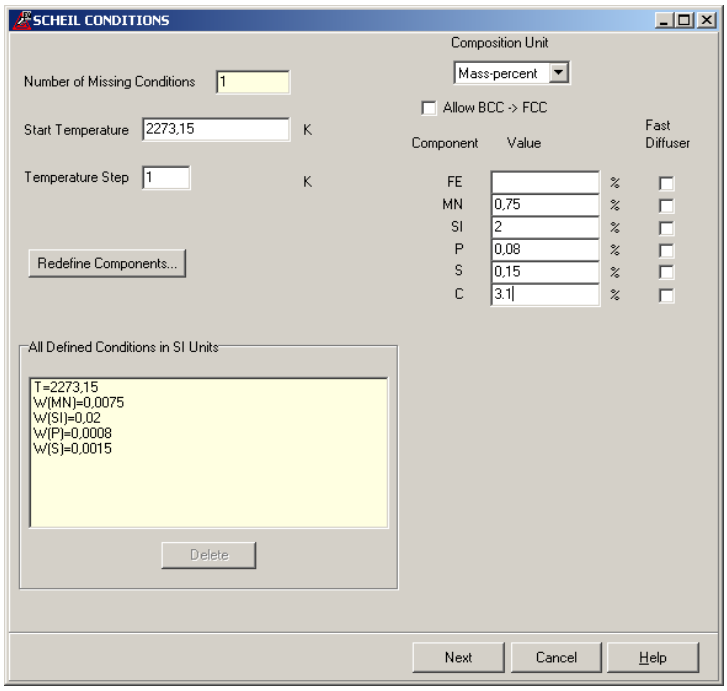
The general procedure start with system that is on the liquidus line at temperature T1 and overall composition x1. The temperature condition is decreased to T2 and the equilibrium is calculated. This gives a certain amount of solid phase(s) formed and a new liquid composition x2. The system with the overall composition equal to x2 would be completely liquid at this temperature. The overall composition is set to x2. This effectively means that the program “forgets” the amount of solid phase(s) formed previously, and that the solid phase(s) will remain at the composition at which it was formed. The simulation is continued from the step 2), and repeated until the lowest temperature where liquid can exist (either all liquid disappear or a certain fraction of liquid remain in the system) is found.

The simulation can easily handle cases where two or more solid phases precipitate at the same time. If it is a eutectic precipitation, all phases will form at each step and the liquid composition will follow the “eutectic valley”. If it is a peritectic transformation, the phase that is no longer stable will disappear from the local equilibrium at the liquid interface. The amount of that phase already formed will not transform as no account is taken of solid phases formed at earlier steps

8.3.2 Scheil Module

The key “Scheil” will start the specialized calculation module. Here, it is possible to quickly simulate the solidification and micro-segregation of an alloy using the Scheil-Gulliver model.
This model assumes full equilibria in the liquid state and of no diffusion in the solid state.

Clicking the key starts a periodic table where the selection of desired database and elements are done.
You can also use the functional key “Material” and select and use a predefined material for the simulation.
For more information about the TABS, Alphabetic List, Periodic Table, Phases, Constituents, see also 6.1.1-4.
Next takes you to the SCHEIL CONDITION window



Functional Keys

Redefine Components	If required, change the component definitions, Redefine the components in the SCHEIL calculation. It is possible to change the components in the SCHEIL calculation.

The number of components must still be the same; components cannot be removed or added only edited. Redefining the components resets the conditions and new conditions may need to be specified.

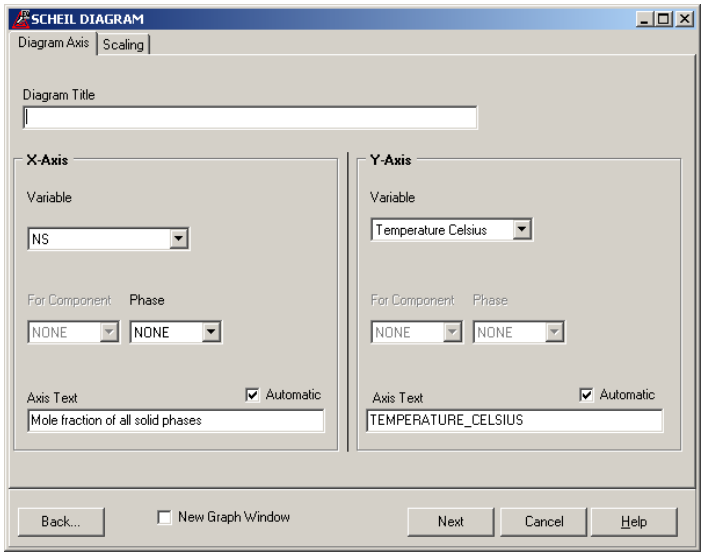
For instance:
CrO2, Fe203 and O could be used as components instead of Cr, Fe and O. Redefining components is rarely used in combination with a SCHEIL-calculation and should thus be used with care.

Check Box

Interstitial	Check this box if the element should be treated as a fast diffusing element.
Allow BCC -> FCC	Allow BCC phase to transform in to FCC phase when it is more stable
Next	Start computation and go to SCHEIL DIAGRAM window

8.3.2.1 SCHEIL DIAGRAM

The SCHEIL DIAGRAM window is a light version of the DIAGRAM DEFINITION window, see section 6.1



Functional Keys

Back…	go to SCHEIL CONDITION window
Next	plot diagram and go to GRAPH window
Cancel	Close window without remembering selection/changes
Help	Show the THERMO-CALC Help page regarding present window/tab

9 SAVING FILES & SCRIPT MANAGEMENT

9.1 Saving files

It is simple to save files in THERMO-CALC. There is a difference between saving equilibria and saving a graphical diagram in THERMO-CALC, a saved graphical diagram does not generally save any thermodynamic equilibrium data.

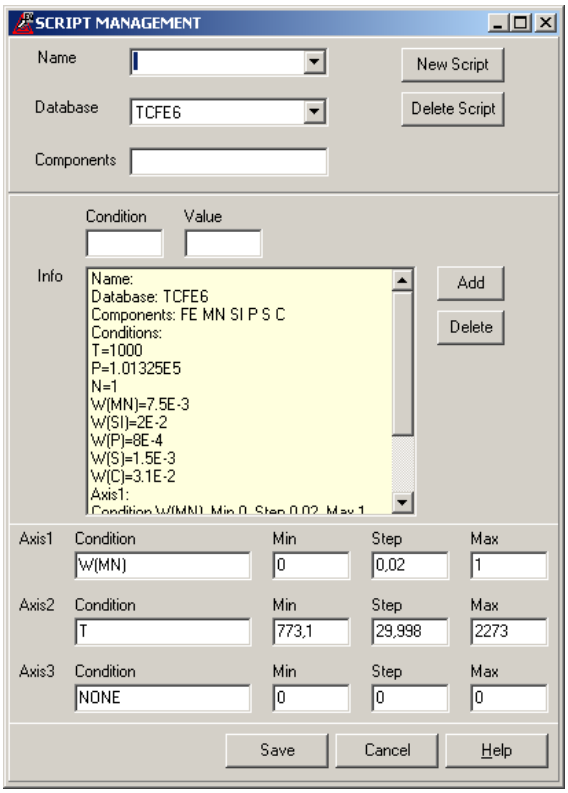
The only exception is when a property diagram is tabulated and saved in format suitable for Microsoft Excel (.xls files). Using this, a diagram may be tabulated and exported to Excel, which enable the user to present the data using the extensive features in Excel.

Calculated initial equilibria and map/step calculations are saved as POLY-3 (.poly3) files.
Use the file menu “save” or “save as” command to save the calculation. The calculation will be saved at the point where the saving is performed. I.e. if the initial equilibrium is saved to a file, the following map/step calculation will not be saved unless a saving is made to the file after the mapping/stepping.

9.2 SCRIPT MANAGEMENT

The Script Management option can be started from

- The menu bar in the MAIN window
- The key in Conditions window
- The key in the Map/Step window



The script management enable management of a previously saved script, edit of a script or a new script can be created.

Fields

Name — Specify a name for the new Script, or select an existing Script to change, in the Name combo box. Every Script name has to be unique. A Script name must be given or specified prior to any action in the window.
After you have created a new Script (i.e., having properly made all the database selection, system definitions, condition definitions and/or axis variable setting) or modified an existing Script, click on the OK button to save the new or modified Script.

Database — Select the database from which data will be read for the defined system, in the Database combo box. Press F2 to get information about the database printed on the THERMO-CALC MAIN window.

Components — Enter the names of the components to be parts of the system in the Component field. The components will be added to the Info field immediately after leaving the Components field. It is possible to go back to the components field and add or remove components.

By default components correspond to chemical elements available in the selected database. However, the uses of some databases (e.g., ION, AQ/TCAQ/AQS, etc.) may require some specially designed elements (such as /- or ZE for electron) to be additionally defined. For vacancy (VA), it is unnecessary to be defined, since the program will automatically handle VA-bearing phases/systems.

Note that a Script does not accept any non-element (such as Al2O3, FeC, C1O2, etc.) in the component definition. If you want to use any non-element as components, you must make appropriate changes in the component definitions of the system afterward, by clicking the Redefine… button on the Components tab of the THERMO-CALC CONDITIONS window.

Condition — Enter a state variable in POLY-3 syntax that is suitable for setting conditions (for example, W(CR)), in the Condition field. Enter the value of the condition (for example 0.18) in the Value field. Click the Add button to add the condition to the Script.

Value — Note that SI-units are used in this window, regardless of the settings in the Units window.

Info — The specified script name, selected database, defined elements, and all of the set conditions and axis variables are listed in the Info field. Delete all the defined elements or any of the conditions by selecting the corresponding line in the list box and click the Delete button. Multiple lines can be concurrently selected by using the ctrl and shift keys. Clicking on the Delete button afterwards will remove all of the selected conditions/elements.

Axis / Condition/ Min/Step/Max — Specify the condition to be used as variable for the axis in the Condition field. It is possible to specify the minimum value, the maximum step size, and the maximum value of the condition in the Min, Step and Max fields, respectively. Axis definitions are not necessary to make a single point equilibrium calculation. To make a STEPPING calculation (of a property diagram) one axis must be defined, and to make a MAPPING calculation (of a phase diagram) two axes must be defined.

Functional Keys

New Script — Click the New Script button to generate a completely new script. After giving the script a unique name, you can select an appropriate database, define system components, initial equilibrium condition, and specify one or two axis variables for the Script calculation.

Delete Script — Click the Delete Script button to delete the currently opened Script. The script will be permanently deleted when the OK button is clicked. Clicking Cancel will leave the script list intact, without deleting the script.

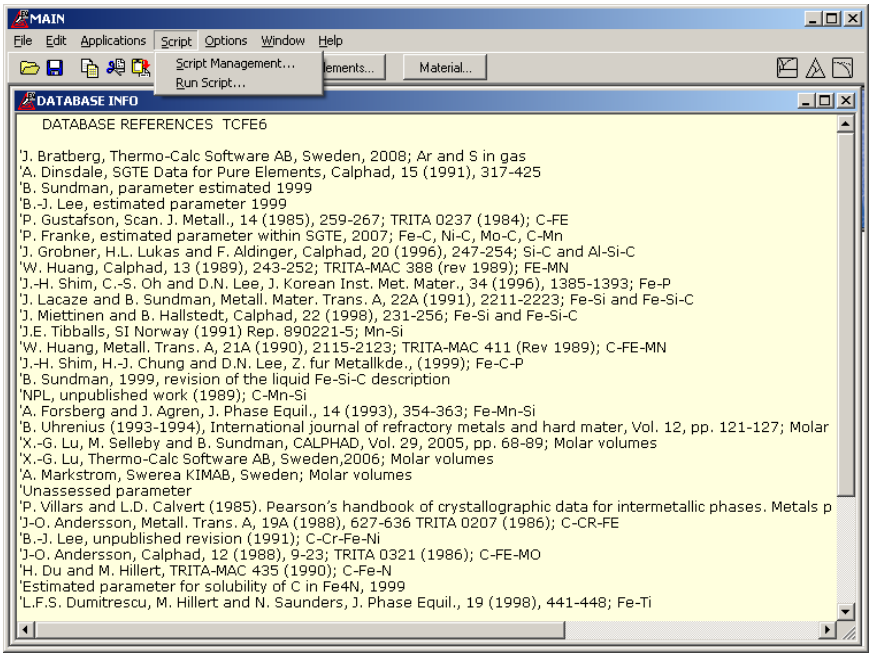
Add / Delete — Clicking the Add button will add the given condition to the Info list box.

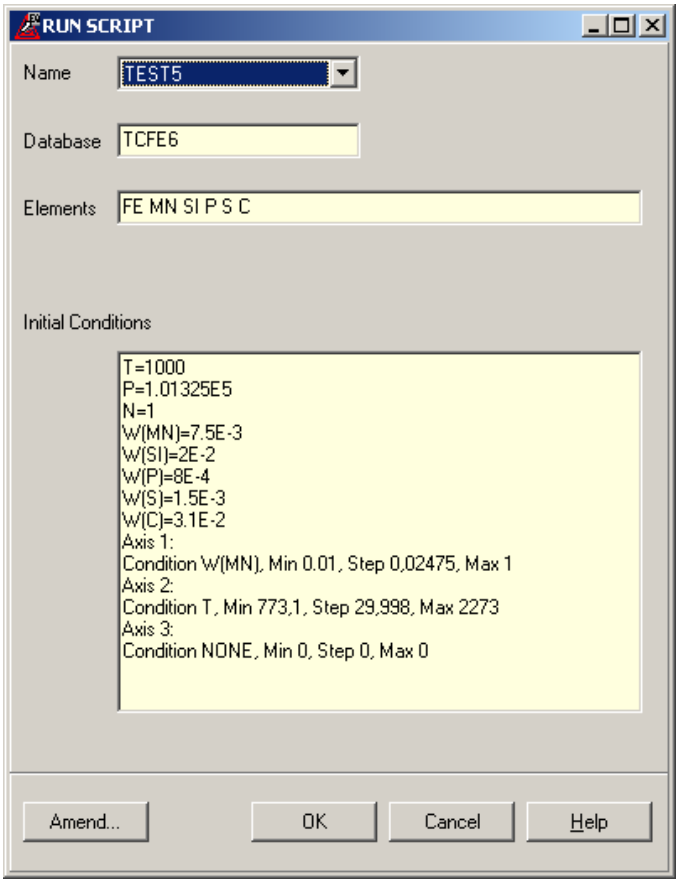
9.2.1 Run Script

A previously saved script can be run by selecting the name of the script and then clicking OK.

If the entered conditions do not allow calculating equilibrium, then the CONDITIONS window will appear.

The CONDITIONS window will also appear if the “Amend” button is pressed in order to change the conditions.





Fields

Name — Use the Name combo box to select a specific script, which has been previously defined, to make a calculation on the Script tab. It is possible to define your own scripts using the Script Management… option from the Script menu on the MAIN window.

Database — Thermodynamic data for the script calculation will be read from the database specified in the Database field.

Elements — The elements defined in the specified script are listed in the Elements field. One of the elements represent the bulk.

Initial Conditions — The initial composition and temperature are listed in the Initial Conditions list box. One or two axes for a step or map calculation may also be predefined. Click on the Amend... button to change these conditions before the calculation.

Functional Keys

Amend — The Amend... button allows changes to be made to the conditions (such as the composition or temperature) before the calculation is made. Click on the button to close the THERMO-CALC RUN SCRIPT window and open the THERMO-CALC CONDITIONS window.

10 OPTIONS

10.1 OUTPUT

These commands affect the equilibrium list on the MAIN window.

You can change them at any moment after opening the MAIN window.
For example, choose the desired option and click on the Equilibrium key of the CONDITIONS window to reorganize the equilibrium result. In this case, only mass-fractions of the stable phases of the composition will be presented in value order in the MAIN window.

The same output will be selected next time Thermo-Calc for Windows is started.

Save Equilibrium to File
To save the equilibrium results in a file, check “Save equilibrium output to file” box and type in the name of the file. If the name field is left empty you will be asked to browse for the file. When you press OK the data is saved.

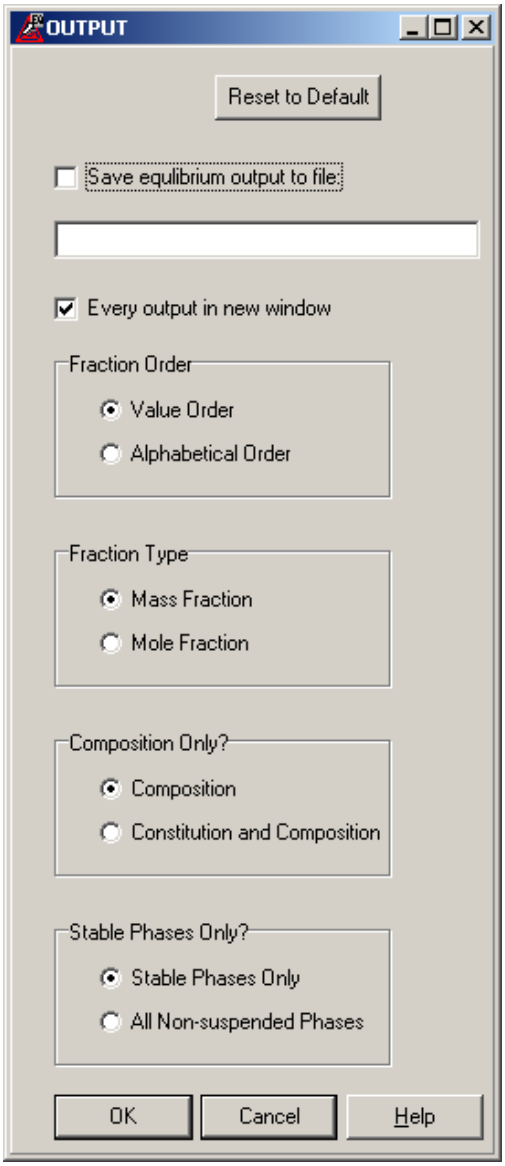
Every output in new window
If the “Every equilibrium output in new window” box is unchecked, the equilibrium results will be listed one after another in the same window.

Fraction Order
Click on the corresponding radio button to choose the way of listing the component fractions of each phase (in either value order or alphabetical order) when showing calculated equilibrium results on the MAIN window.

Fraction type
Click on the corresponding radio button to choose if the output should be in either mass fraction or mole fraction when listing calculated equilibrium results on the MAIN window.

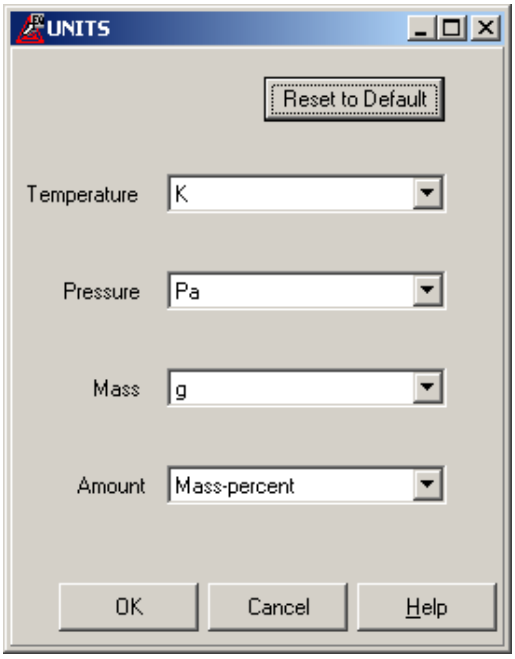
Composition Only?
Click on the corresponding radio button to choose if listing only the composition or both the constitution and the composition of calculated equilibrium results on the MAIN window.

Stable Phases Only?
Click on the corresponding radio button to choose if listing only the stable phases or all non-suspended phases of calculated equilibrium results on the MAIN window.



10.2 UNITS

In the UNITS window you can select the units you want to use in your calculations.



Functional Key

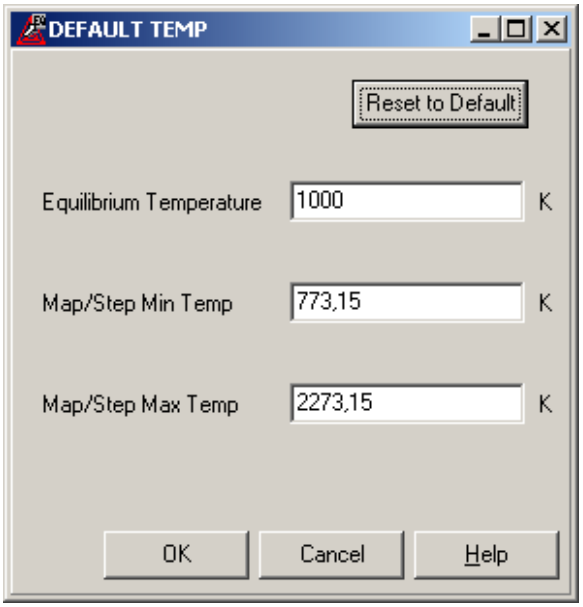
Reset to Default	Clicking the Reset to Default button will reset all the units to their THERMO-CALC-factory assigned default values (mostly SI-units): Temperature to Kelvin, Pressure to Pascal, Mass to gram, and Amount to mass-percent.

Fields

Temperature	Kelvin (K), Celsius (C), or Fahrenheit (F),
Pressure	Pascal (Pa), bar, or atmosphere (atm)
Mass	Kilogram (Kg) or gram (g)
Amount	moles, mass, mole percent, mass percent, mole fraction, or mass fraction

10.3 DEFAULT TEMPERATURE

In the DEFAULT TEMP window you set defaults for STEP and MAP calculation.



Functional Key

Reset to Default	Clicking the Reset to Default button will reset settings to their THERMO-CALC-factory assigned default.

Fields

Equilibrum Temperature	Default for single equilibria
MAP/STEP Min Temp	Enter default lowest temperature during MAP and STEP
MAP/STEP Max Temp	Enter default highest temperature during MAP and STEP

Note that the temperature unit are set in the UNITS window

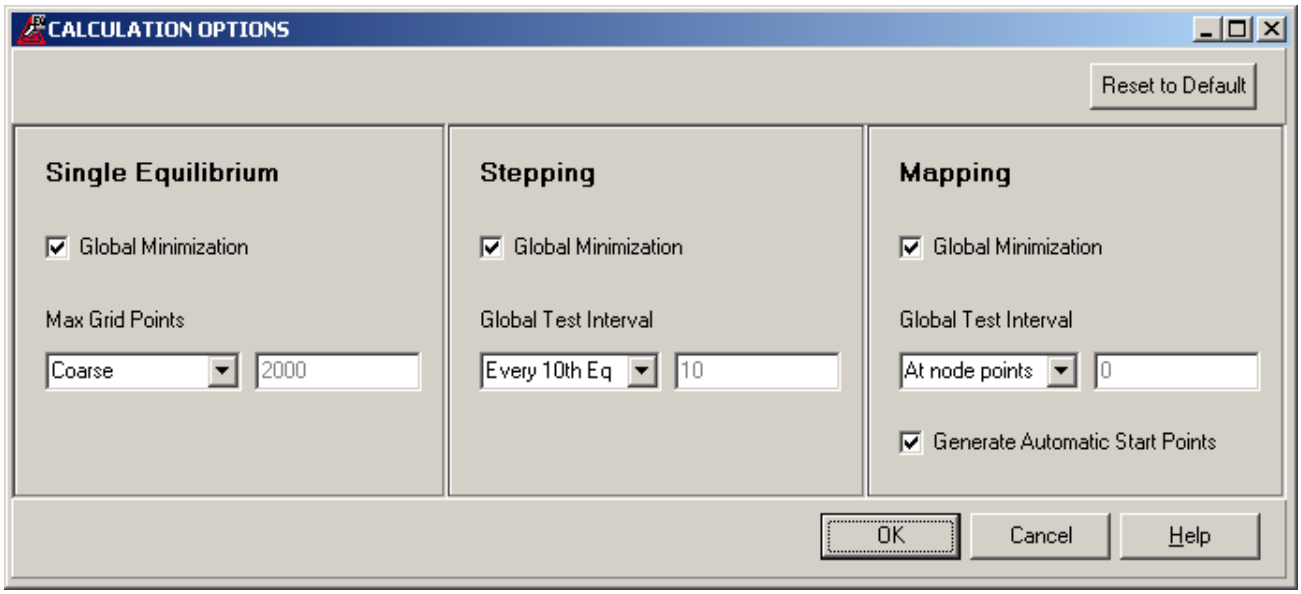
10.4 GLOBAL MINIMIZATION

Here it is possible to specify if the global minimization algorithm shall be employed by Thermo-Calc when calculating Single Equilibrium or not.

The maximum number of grid points when searching for the global minima can also be specified.

The Global Minimization is turned on by default. The settings here will affect all calculations and will be saved, i.e. the settings will be the same after restarting Thermo-Calc for Windows.

Use the Global Minimization check box to turn global minimization on and off.



Fields

Max Grid Points — Select the maximum number of grid points for the global minimization.

Choose between predefined grid points:

Coarse	2000
Medium	20000
Fine	200000
Custom	to select a number of your own choice.

Global Test Interval — Select the interval for testing with global optimization during mapping and stepping
Every 10th
Always
Custom
At node points (Only for mappings)

Check boxes

Global minimization — Select if to (to not use any global minimizations during Single Equilibria, Stepping, and Mapping.

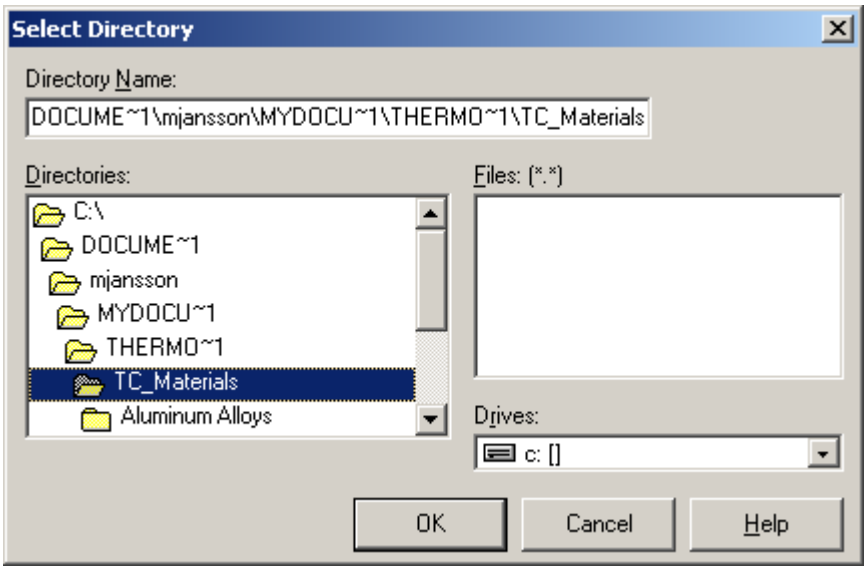
Generate Automatic Start Points — If unchecked mappings will only start from a single equilibria, checking leads to a few start points all over the mapped diagram. Automatic Start Points uses more time but might make mapping more complete reducing the chance of missing a line.

Functional Key

Reset to Default — Clicking the Reset to Default button will reset settings to their THERMO-CALC-factory assigned default.

10.5 OPTIONS DEFAULT MATERIALS FOLDER

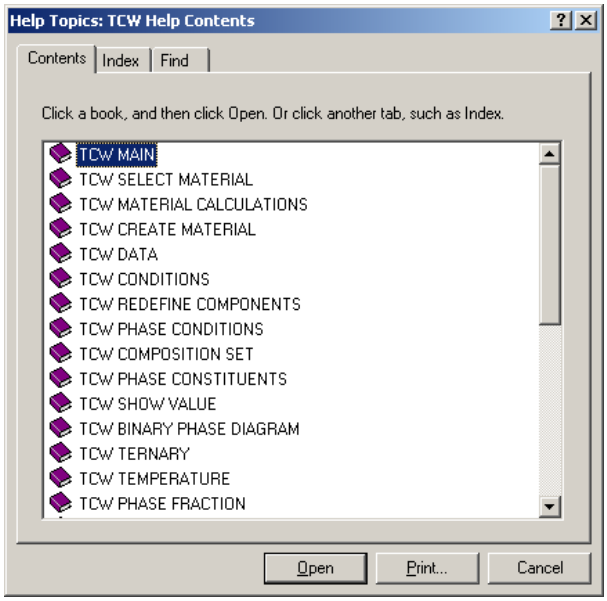
Here the path to the folder containing the different, default or user specified, materials can be set.



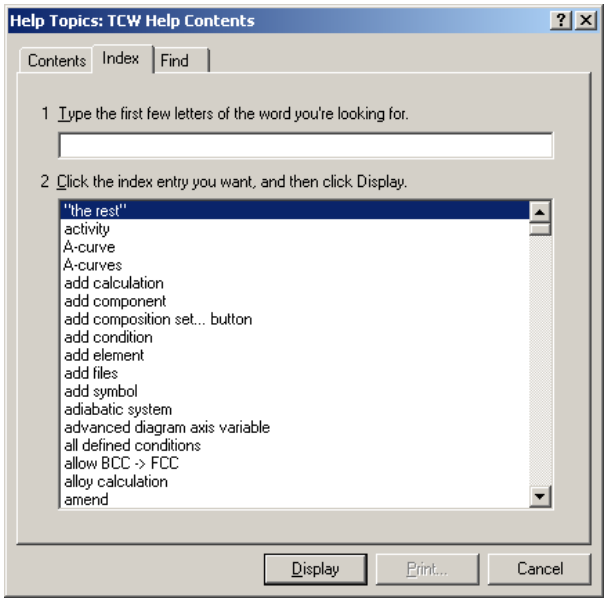
11 HELP

The Thermo-Calc Software Help function will make it easy for you to find helpful tips and solutions to how to operate the software. You can also use F1 in fields and areas while running the program or you can right click while having the mouse pointer over the object of interest.

11.1 TAB: CONTENTS

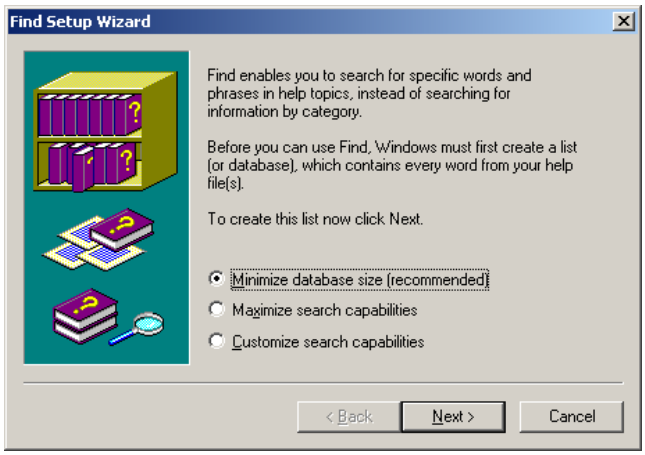


11.2 TAB: INDEX

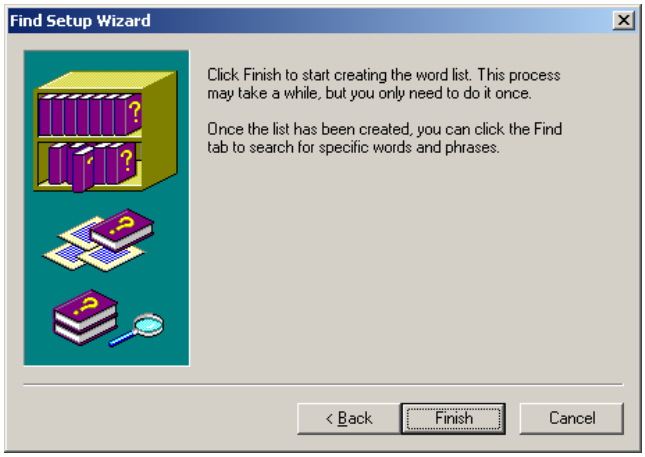


11.3 TAB: FIND

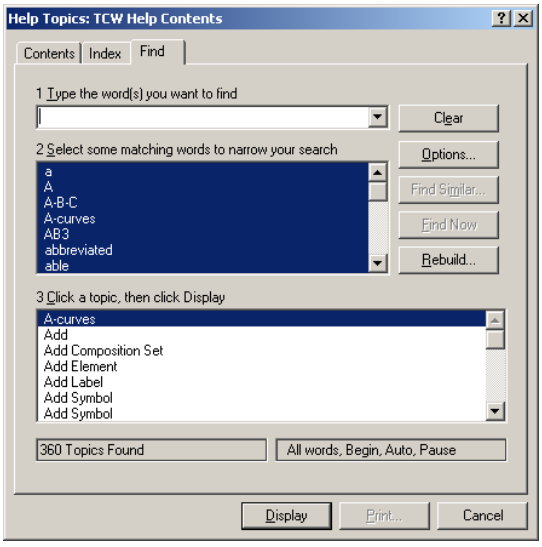
The first time you go to the Find tab you go through the “Find Setup Wizard”



Select one of the first two, if you are not an expert in Windows, then press Next.

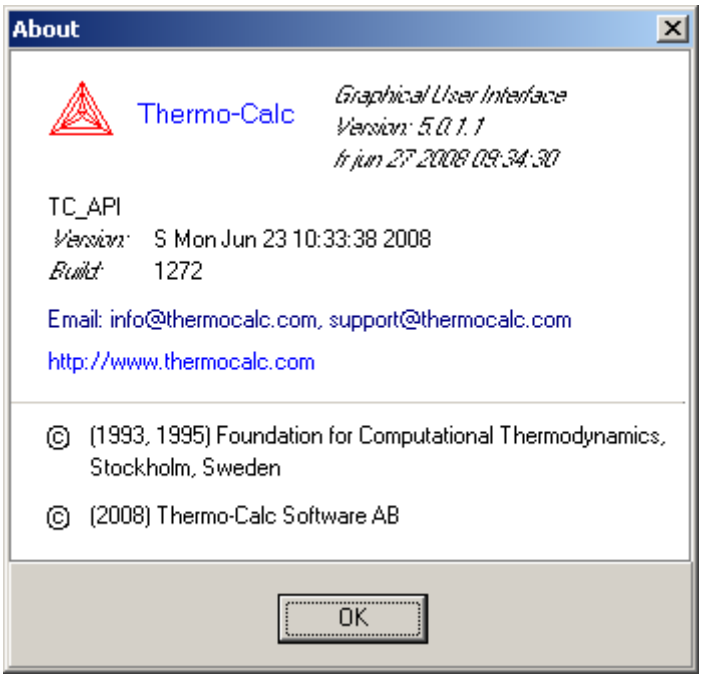


Press Finish and wait for a while to finally get to the Find tab. Consequent visits to the Find Tab will directly take you here



11.4 ABOUT

Gives you information about your license and the version of the software.



11.5 THERMO-CALC SOFTWARE SYSTEM

Opens the user's guide TC_Software_System.pdf
This document is the main document in the Thermo-Calc user's guide and contains links to all the other user's guides; TCC, TCW, DICTRA , and the programming interfaces. It also contains basic information regarding thermodynamics and a description of all state variables that can be used in Thermo-Calc.

11.6 USERS GUIDE

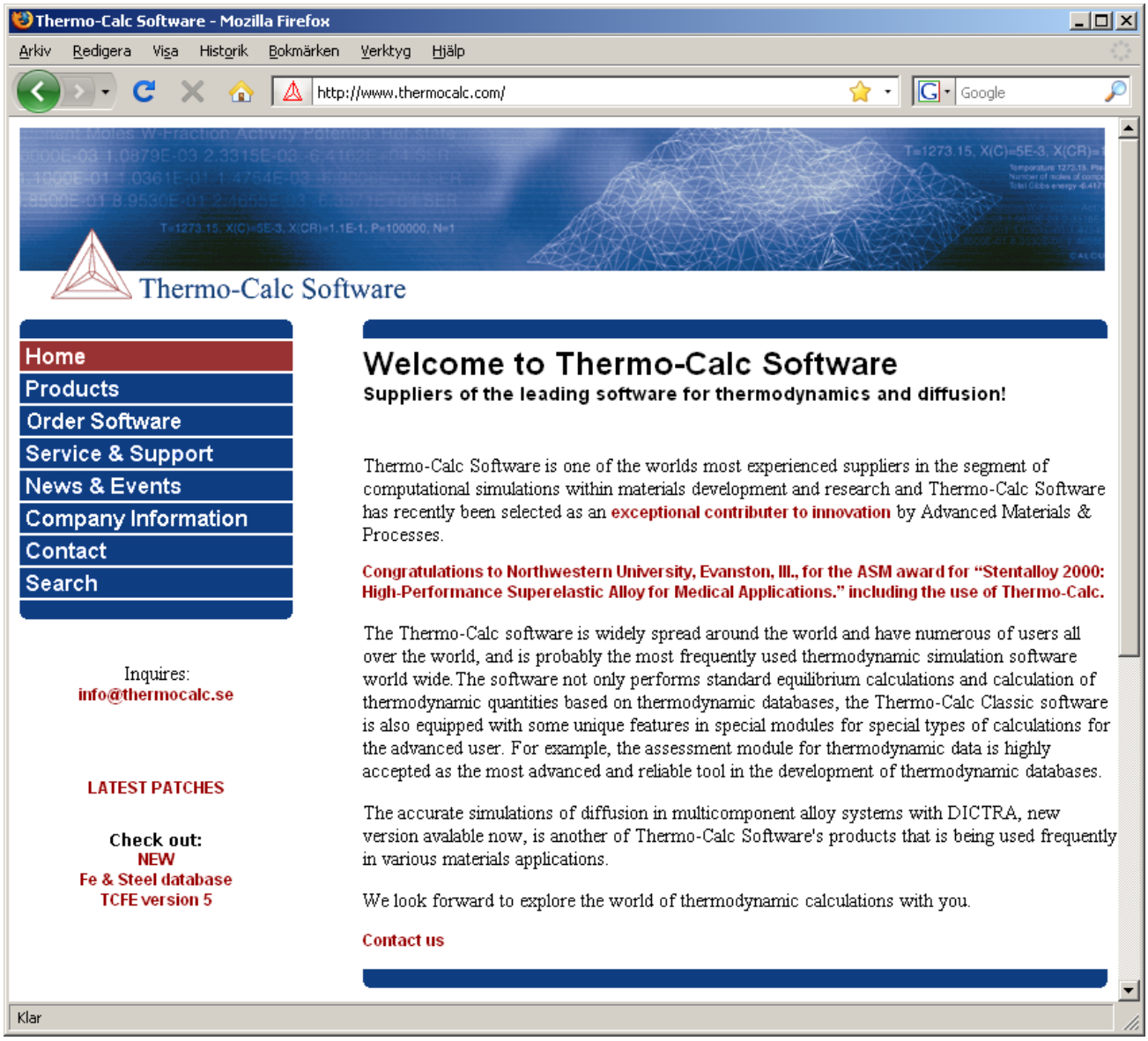
Open this document, the User's Guide.
TCW5_UsersGuide.pdf

11.7 EXAMPLES

Open the examples collection for this software, Thermo-Calc.
This document contains many different detailed examples on setting up and doing calculations with Thermo-Calc.

11.8 THERMO-CALC SOFTWARE HOMEPAGE

Link to the Thermo-Calc Software website: www.thermocalc.com



12 FAQ: TROUBLESHOOTING

In order to get immediate help on a particular topic, press the right mouse button, the F1 key and/or the help button at the bottom of any window.

Other Frequently Asked Questions (FAQ) are listed and answered below. The questions are organized into separate categories by window title. See another helpful list by clicking on things to remember.

12.1 FAQ: GENERAL INFORMATION

6.1.1 QUESTION: How do I find out about THERMO-CALC updated versions or databases that might be suitable for me?
ANSWER: Check out the homepage www.thermocalc.com for updates, patches under NEWS, additional products and services.

6.1.2 QUESTION: What is the maximum number of elements that THERMO-CALC can compute in one calculation?
ANSWER: 20. You will be warned if you attempt to select a larger number.

12.2 FAQ: MAIN WINDOW

6.2.1 QUESTION: How do I save my conditions and equilibrium in order to work on it later?
ANSWER: Click on the save button or the file menu/save any time during the calculation. Only calculations made before the saving will be saved. If you save immediately after the equilibrium calculation, no mapping/stepping will be saved in that file. To save the mapping/stepping calculation, save the file after the mapping/stepping. The final diagram can be saved in many different formats to be used in other programs.

6.2.2 QUESTION: How can I change the units in THERMO-CALC MAIN window? I changed the pressure and temperature units on the THERMO-CALC UNITS window and then I pressed the equilibrium button and no change appears.
ANSWER: The units in the THERMO-CALC MAIN window can only be changed between mole and mass fraction using the Options/Output menu. THERMO-CALC always calculates and presents the information in SI units and fractions. The THERMO-CALC UNITS window only adjusts the appearance of the input on the THERMO-CALC CONDITIONS window.

12.3 FAQ: DATA WINDOW

6.3.1 QUESTION: What does the designation FE#1, C#2 etc. mean in Constituents tab of THERMO-CALC MATERIAL window?
ANSWER: The number after the hash (#) denotes the number of the sublattice. FE#1 thus means the element iron on the first sublattice. In complex phases the same element may appear in several different sublattices

12.4 FAQ: CONDITIONS WINDOW

6 QUESTION: How do I change the reference state
ANSWER: Click on the set reference state tab on the THERMO-CALC CONDITIONS window. Click on a particular component and then choose the reference state phase, temperature, and pressure

7 QUESTION: Why can THERMO-CALC not compute an equilibrium based upon the conditions that I have, with 0 degrees of freedom?
ANSWER: Check your conditions, this happens because some combination of conditions might cause the equilibrium calculation to fail. For instance your mass- or mole-fractions might be larger than 1. It is recommended to start with conditions on temperature, pressure and over-all composition. After this has succeeded it is easier to calculate an equilibrium with “advanced” conditions, such as activities/chemical potentials, composition in specific phases etc.

8 QUESTION: Why does Thermo-Calc for Windows sometimes set some of the conditions automatically in the CONDITIONS window?
ANSWER: Thermo-Calc for Windows tries to be as user friendly as possible. This implies that the program already has some automatic default values in order to facilitate the calculation process. These values, however, can be changed.

9 QUESTION: What is the THERMO-CALC Conditions/Phases/Phase Conditions button for?
ANSWER: This button allows conditions to be set for particular phases. For instance it is possible to set a condition that the FCC phase should contain 15wt% of Cr.

10 QUESTION: What is the difference between mass-fraction/mass-percent and mole-fraction /mole-percent?
ANSWER: A factor of 100: 40 mass-percent is 0.4 in mass-fraction.

12.5 FAQ: MAP/STEP DEFINITION WINDOW

11 QUESTION: Why can't I choose any variable as axis variable in the map/step definition?
ANSWER: In the map/step calculation it is only possible to use conditions from the initial equilibrium as axis variables. If you have calculated an initial equilibrium with conditions on temperature (T), pressure (P), weight-fraction of Cr and C (w(cr) and w(c)) and size of system (N), then these five variables (T,P,N,w(cr) and w(c)) are the only possible axis variables. For convenience they are listed first in the Variable pull-down menu in the THERMO-CALC MAP/STEP DEFINITION window. After the map/step calculation it is possible to plot diagrams with other axis variables, which may be selected using the THERMO-CALC DIAGRAM DEFINITION window.

12 QUESTION: In my calculation of Gibbs energy vs. Mole-fraction diagram, why does the x-axis (mole-fraction) only go up to 0.8?
ANSWER: Firstly it is possible that you have defined your calculation in a way that limits the x-axis. For instance stepping a Fe-0.2Cr-Ni alloy from 0 to 1 in weight fraction of Ni would cause the x-axis to end at 0.8 Ni since the alloy always contain 0.2 Cr and Ni simply replaces Fe in the stepping (conditions on T,P,N,w(cr) and w(ni), w(ni) as axis variable). It is also possible that this is caused by phases that have a limited solubility range and are modeled accordingly, which can cause GM-curves to stop at certain compositions.

13 QUESTION: What is the difference between function and variable in the User Symbols tab?
ANSWER: There is a difference that is inherited from Thermo-Calc Classic: variables are updated only when called upon, while functions are updated in every equilibrium calculation. When using THERMO-CALC: use function!

12.6 FAQ: DIAGRAM DEFINITION WINDOW

15 QUESTION: What is GM in the axis box in the THERMO-CALC DIAGRAM DEFINITION window?
ANSWER: G depends on what you plot- GM stands for the Gibbs energy per mole, GW is the Gibbs energy per gram, etc.

12.7 FAQ: GRAPH WINDOW

16) QUESTION Why can I not print out the final diagram?
ANSWER Ensure that Ghostscript is installed on your computer. If not, install it from the THERMO-CALC CD

17) QUESTION Why are all of the phase boundaries not shown on my phase diagram?
ANSWER This problem usually results from the initial equilibrium calculation since the diagram is often calculated with the initial equilibrium as the starting point on the final diagram. The diagram cannot be calculated in its entirety if not all phase boundaries are connected. Try making the calculation again by starting with the initial equilibrium in a two-phase region close to the region where not all phase boundaries are shown.
Another alternative is to check the Generate automatic start points box. The new calculation will take longer time, but normally all disconnected lines will be found.
Finally, you could also try using a wider calculation interval on your axis-variables since this increases the possibility that the phase boundaries cross each other.

18) QUESTION Why do I get strange results when I plot per volume?
ANSWER Most of the databases have limited pressure and volume dependent data. Using this option may give an unreliable result.

12.8 FAQ: OUTPUT

19) QUESTION What does the THERMO-CALC OUTPUT window control?
ANSWER This window allows you to manipulate the format of the output from an equilibrium calculation in the THERMO-CALC MAIN window.

12.9 FAQ: GLOBAL MINIMIZATION

20) QUESTION When and why should I turn off the global optimization?
ANSWER To ensure that the calculated minima correspond to the global minima of the system global minimization should be turned on. However the computational time is increased when global minimization is turned on, and in some cases it may be of interest to decrease the computational time.

12.10 FAQ: ERROR MESSAGES

21) QUESTION What does Error in CFCETH- ERROR COMPUTING EQUILIBRIUM mean?
ANSWER This error message appears when an equilibrium calculation has failed.
See also question 7.

22) QUESTION What does ERROR IN QSETAX: CANNOT SET NEW AXIS CONDITIONS AS DEGREES OF FREEDOM ARE ZERO mean?
ANSWER This message appears when you have tried to specify an axis variable, which is not a condition in your initial equilibrium. See also question 11.

12.11 IMPORTANT THINGS TO REMEMBER

In addition to this THERMO-CALC Users' Guide four different external documents may be useful for the THERMO-CALC user.
Links to all documents can be found as bookmarks to the left in this window and for the linking to work all documents must remain in the same folder as the THERMO-CALC Users' Guide. Below follows a short description of the four external documents supplied with this manual.

The "Thermo-Calc Software System" manual contains basic information regarding thermodynamics and a description of all state variables that can be used in Thermo-Calc.

The "Thermo-Calc Database Guide" contains a description of the available databases. Some information regarding the database format is also available.

In the "Dataplot Users' Guide & Examples" the DATAPLOT graphical language is discussed. This may be useful for editing experimental data files (.exp-files).

Finally a list of references is supplied as an external document to this THERMO-CALC Users' Guide. The reference list contains only a small part of all reports concerning Thermo-Calc that have been produced the last 25 years. Although far from complete, the reference list covers model development, database development and applications of the Thermo-Calc software package.

The following is a list of key aspects that are worth keeping in mind while using THERMO-CALC. Refer to this list, the help functions, and the troubleshooting section when you are having difficulties using the program.
If none of these resources are adequate and you have a valid M&SS, Maintenance & Support Subscription, further help can be obtained by sending an email to **support@thermocalc.se.**

- The number of degrees of freedom (number of missing conditions) must be zero to calculate an initial equilibrium.
- The map/step calculation variables need to be consistent with the calculated initial equilibrium in order to calculate the final diagram from the initial conditions.
- The initial equilibrium is often the starting point for the map/step calculation. It is useful to start a map/step calculation in a two-phase region. Use automatic start points to help ensure calculation of the entire diagram.
- Map/Step an area larger than the final phase diagram needs to display. It is better to calculate a larger range to help obtain the phase boundaries of entire diagram.