

New releases from Thermo-Calc Software

It is again our pleasure to distribute new software versions from Thermo-Calc Software to all of our maintenance and support subscribers around the world.

Our main ambition and focus in developing these new versions of Thermo-Calc, the TC-Programming Interfaces and DICTRA has been to increase the robustness and reliability for all type of calculations. As you may recall, a major improvement for the previous version was the implementation of a new global minimization strategy, which ensures that truly stable phase equilibrium is calculated under given conditions. In the new version this technique has not only been further improved, but also extended for use when stepping along an axis variable, or when mapping in two or more axis variables. This work has been very extensive, but we believe also very successful. We feel confident that you will come to the same conclusion.

On the following pages of this document you will find brief descriptions of the main new features introduced in the respective software products. For more details we recommend that the new user's guides are consulted.

Enclosed you will find an installation CD containing the new versions of our software and databases. The installation CD contains:

- Thermo-Calc Classic version S
- Thermo-Calc for Windows, TCW version 5.0
- DICTRA version 25
- TQ-Interface version 7.0
- Thermodynamic databases
- Kinetic databases

Also enclosed is an installation guide that we recommend you to follow. Please only choose to install the products for which you have a valid maintenance & support subscription.

A new license file is required in order for running the new software versions. In most cases this new license is included on the CD. The so-called "HostID" in your new license should be the same as in your present license file. Please make sure this is the case.

Note that with this release we introduce a new license system based on Sentinel RMS from SafeNet. If you have a network installation and need instructions for starting a license manager, then please consult the documentation we have prepared for this purpose.

Our development efforts continue and work has already been started on the next versions of the codes with the intention to ship the next releases within 12-18 months.

Enjoy using your new software!



New Features Common to Thermo-Calc Classic ver. S and Thermo-Calc for Windows, TCW ver. 5

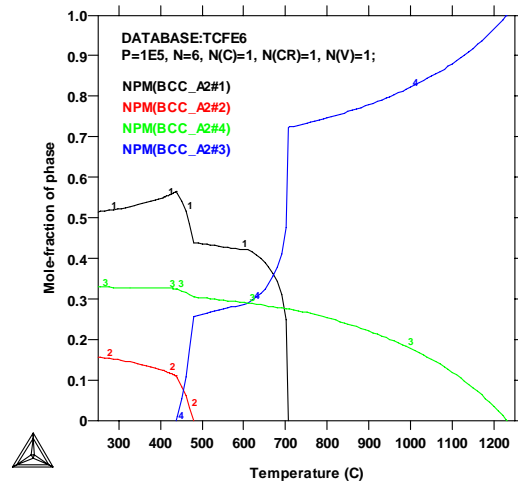
Improved Global Minimization

A major improvement in the previous version of Thermo-Calc was the implementation of a global minimization routine which ensures that truly stable phase equilibrium is calculated under various given conditions. The efficiency of this technique has been further improved for the new version which results in more robust and time-efficient calculations.

New Stepping and Mapping Routines

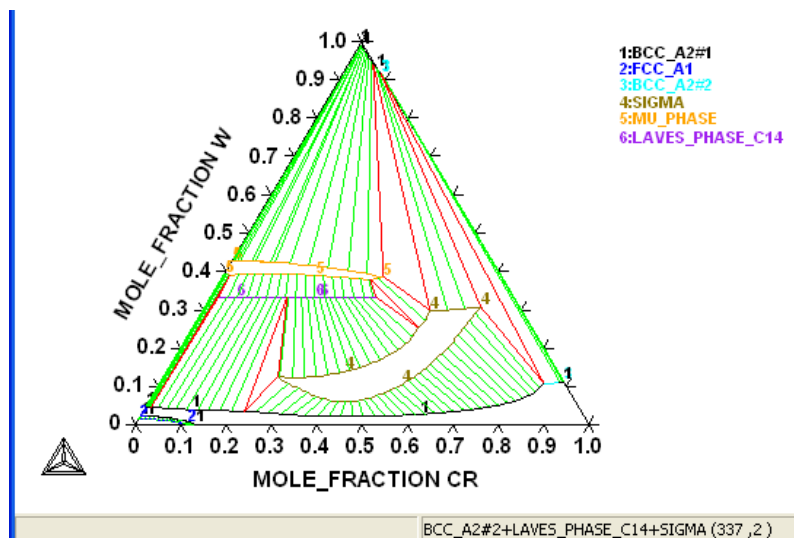
Global minimization is now applied also by default during the stepping and mapping operations. The routines for stepping and mapping have been completely rewritten for this purpose. Another change is that multiple starting-points will by default be provided automatically for mapping. All these improvements have resulted in more stable and in particular more reliable calculations.

The figure on the right is an example demonstrating how the new stepping procedure in ver. S automatically captures a BCC phase splitting metastably into 4 BCC phases in the Fe-Cr-V-C quaternary system, with two of them being Fe-rich and Cr-rich alloys and the other two being a (Fe,Cr)-rich alloy and a cubic V-rich carbide VC3-x.



Improved Ternary Module/Application

As already mentioned global minimization is now by default used during mapping calculations, and this is also the case when calculating ternary phase diagrams using the ternary module inside TCC, or alternatively the ternary application present in TCW. This type of calculation is now very robust.



The figure on the left shows a calculated isothermal section for the Fe-Cr-W system calculated at 1100 °C. Even though this system contains a miscibility gap as well as an isolated γ -loop the complete diagram is automatically calculated without prior knowledge.



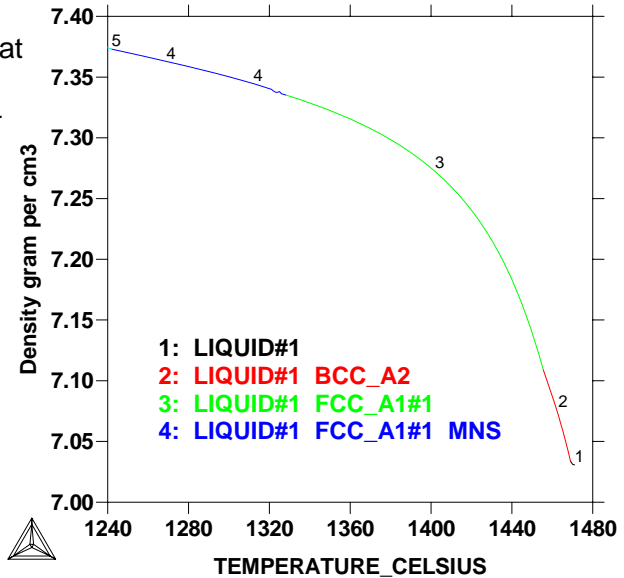
Extensions in the Scheil Module/Application

When using a database (such as TCFE6) that contains volume data (*i.e.*, molar volume, thermal expansivity, and compressibility), then the improved SCHEIL Module/Application can plot diagrams using one of four additional variables calculated during the solidification process.

The four variables are CP/BCP – Apparent heat capacity per mole/gram, NV/NV(ph) – Molar volume of the system or a phase, DS/DS(ph) – Average density of the system or a phase, and BT – Apparent volumetric Thermal Expansion Coefficient of the system.

In addition, it is now also possible to plot site-fractions for elements, as well as normalized element distribution in different phases.

The figure to the right shows the calculated average density in a tool steel (ASTM A681) followed by a Scheil simulation.



Thermo-Calc Classic ver. S – Specific Changes

SYS Module

A new command SET_TC_OPTIONS has been introduced that allows a user to some extent tailor her/his own default settings, *i.e.* 1) global minimization can be turned off, 2) frequency of global test during step/map can be set, and 3) the automatic creation of start points in mapping may be turned off. This command is only intended for expert users.

TDB Module

The CASE directive in TDB files is now working. It makes it possible to have additional TDB, GES or POLY commands executed depending on the user selection of elements, species or phases.

In order to handle chemically-ordered solution phases with partitioning (in 4-substitutional sublattices), the phase-type option F for ordered FCC/HCP phases has been improved and simplified, and the phase-type option B for ordered BCC solution phases has been implemented.

The TDB module can now selectively retrieve only the functions which are necessary for a defined system when reading from a database that has functions stored in its setup file or SEQ sequential function file.



GES Module

The *Four Substitutional-Sublattice Ordering Model* (which requires that a solution phase has 4 sublattices for substitutional ordering and can additionally have an interstitial sublattice) has been extended for chemically-ordered FCC (or HCP) solution phases (*i.e.*, with the phase-type F), and has also been implemented for chemically-ordered BCC solution phases (*i.e.*, with the new phase-type B). An additional advanced feature with the phase-type options F and B is that a composition set that represents the solution phase will have a suffix that is automatically added to its phase name in listings of equilibrium calculations. Such suffix indications can be: `_L12` or `_L10` for ordered FCC, or `_A1` for disordered FCC; `_B2`, `_B32`, `_D03` or `_L21` for ordered BCC, or `_A2` for disordered BCC; `_D019` and `_B19` for ordered HCP, or `_A3` for disordered HCP.

The `MIXED_EXCESS_MODELS` option for amending `EXCESS_MODEL` of binary interactions, as well as the `TOOP_KOHLER` model for amending `TERNARY_EXTRAPOLT` method have been improved.

POLY Module

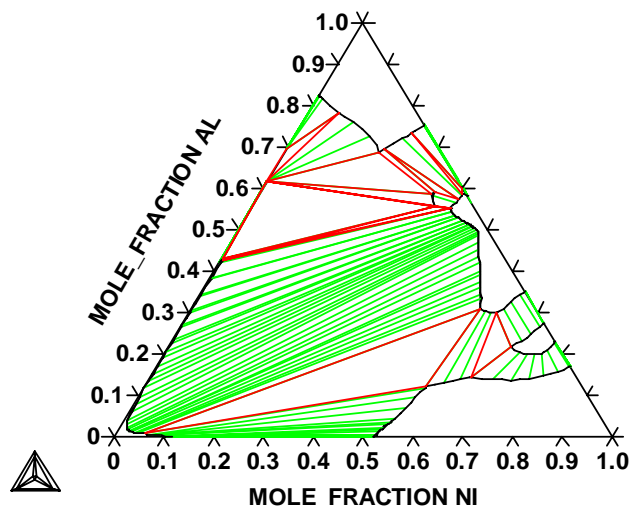
The efficiency in the global minimization routine has been further improved, which makes it possible to apply the technique during stepping and mapping.

A new `STEP NORMAL` routine now uses global minimization to guarantee that the current equilibrium is the lowest energy state and that this is also true at every phase change.

A new `MAP` routine has also been implemented which adopts global minimization to guarantee that the current equilibrium is the global minimum and that is also true at every node point.

For single point, stepping and mapping, the new global minimization routines can also be turned off using the command `ADVANCED_OPTIONS` that supersedes the old `SPECIAL_OPTIONS` command.

The figure on the right is demonstrating the new improved mapping capability. The diagram calculated displays a ternary isothermal section for the Al-Cr-Ni system at 1100 °C. The complexity in this case stems from the modelling of the A2 (BCC) and B2 (CsCl) phases, which have been made using a single Gibbs energy description.



Note the new `MAP` command will by default generate several equilibrium points to be used for starting points. Users may still select to start from one (or several) specific starting points by using the command `ADD_INITIAL_EQUILIBRIUM`. This may result in a faster calculation.

POST Module

In the `SET-PLOT-OPTION` command additional options "Always initiate ..." and "Always solid line" have been added.



For the option "Always initiate ..." the default answer is Y, which means that POST will reinitiate automatically whenever the workspace in POLY has been changed on return. If answered N the same plot axis will be kept even if the workspaces in POLY has been read or written to file. The N answer is useful, for example, if one has several sets of POLY files with the same calculation but for different set of model parameters.

PARROT and ED-EXP Modules

The command SET-SCALED-VARIABLE which allows specifying a lower and upper limit for an optimizing variable now works correctly.

In the POP file and in the EDIT module one can use a new type of symbol in the ENTER-SYMBOL command for ordered phases which have type F or B. This is called INTERNAL and can be specified as L12, L10, D019, B19, D03, L21, B2 or B32 and in addition a phase and composition set must be specified. The symbol value will be zero if the phase is not ordered according to the specification; otherwise it will have a positive value depending on the degree of order, with a maximum value of unity. This is useful when optimizing ordered phases as the order may change during the optimization.

The LIST-RESULT command has a slightly modified option D to list all experiments, including those with fulfilled inequalities which are suppressed with the default option C.

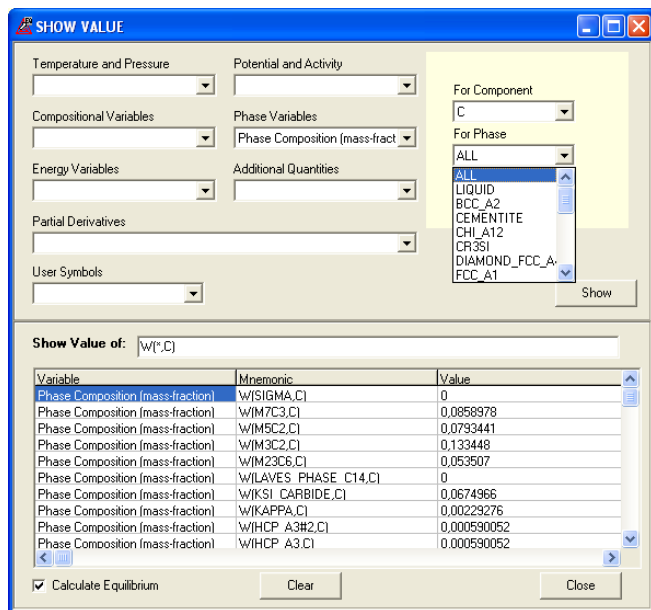
Normally GLOBAL minimization of the equilibrium is turned off during optimization. However, it is possible to turn it on for individual experiments with the ADVANCED-OPTION GLOBAL_MINIMIZATION command.

Thermo-Calc for Windows, TCW 5 – Specific Changes

Extracting result using pull-down menus

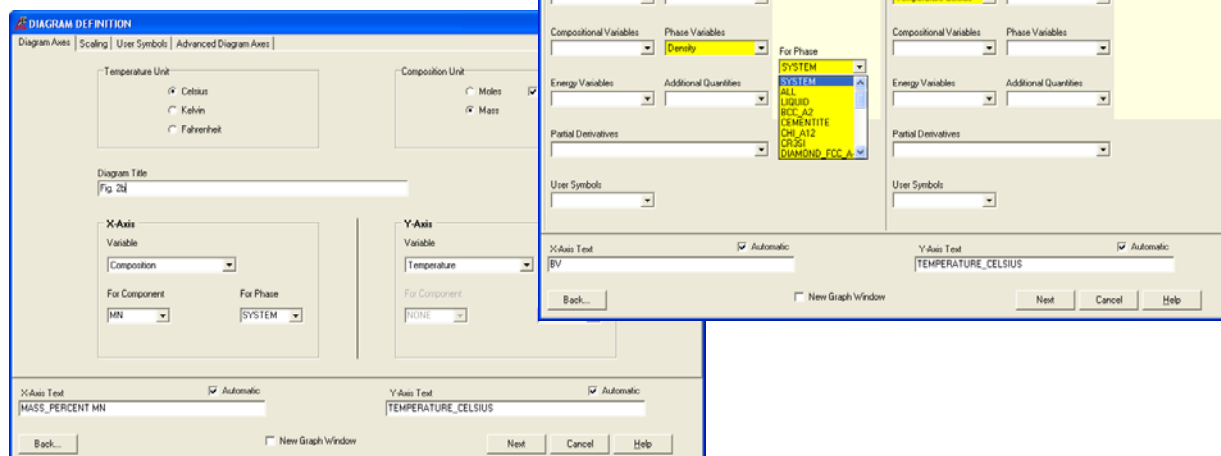
The Show Value Window has been modified in order to allow the user to specify the variable to evaluate from pull-down menus. This will make it easier for users to quickly have an overview of the vast number of variables available, without any knowledge of Thermo-Calc Mnemonics.

It is still possible to directly type in the variable in the same manner as in the earlier versions, i.e. by typing the Thermo-Calc Mnemonic for a specific variable. By typing in the variables directly it will in addition be possible to evaluate several variables simultaneously provided they are separated by a semicolon, i.e. “;”.



New Diagram Definition Window

Variables to be plotted on a diagram are now defined in a somewhat different manner, with advanced variables placed under the “Advanced Diagram Axis” tab. Rather than placing all the variables in a long list they have now been divided in several categories in order to give the user a better overview.



New Functionality Common to all Thermo-Calc Programming Interfaces

There are no specific new changes made to any of the three programming interfaces provided by Thermo-Calc Software, i.e.

- ✓ TC-API ver. 5
- ✓ TC Toolbox for MATLAB ver. 5
- ✓ TQ-Interface ver. 7

but all of them benefit from the improvements made inside the Thermo-Calc core.

Improved Global Minimization

Improvements in the global minimization technique will result in more robust and efficient convergence during equilibrium calculations. Since global minimization is not the default option with any of the programming interfaces, then as with the previous versions the user has to specify that the global minimization technique should be enforced using the command “tc_set_minimization” (TC-API and TC Toolbox for MATLAB) or calling the subroutine TQCEG (TQ-Interface).

New and Updated Examples

All existing examples have been updated, and some new examples have been added.

DICTRA version 25 – New Functionality

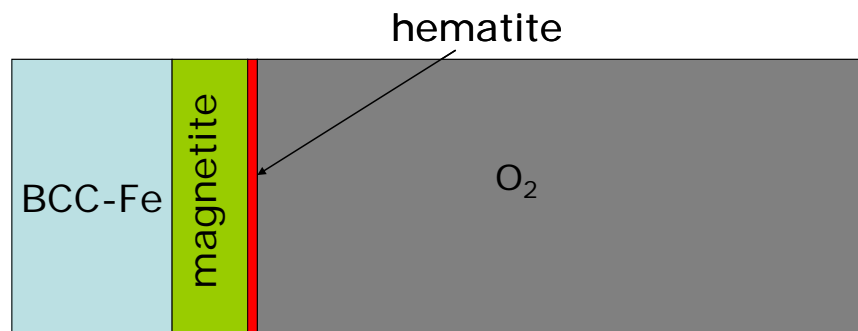
Improved convergence

The new version has an improved procedure for the generation of automatic start values for activities/potentials at a moving phase interface. This has resulted in improved simulation stability for so-called moving phase-boundary problems.

Diffusion models for complex phases

In the new version of DICTRA we consider diffusion of elements, instead of species as was the case in earlier versions. This is a large change that has been introduced in order to obtain a better treatment of diffusion in phases that are modelled with the same specie on several sublattices, e.g. phases showing chemical ordering, as well as to manage ionic phases modelled with charged species, e.g. Cr^{2+} , Cr^{3+} etc.

This means that it is now at least in principle possible to simulate oxide growth on a steel surface as indicated by the set-up in the figure on the right. It should be noted though that there is very little mobility data assessed for oxides.



A new example i3 has been added to visualize the structure for modeling mobility data in ionic phases, and the growth of an oxide layer on top of iron surface.

The diffusion model used for stoichiometric phases has been rewritten, and due to a generalized treatment, the fluxes for all elements for which mobility data are available are now calculated, and also used in the simulation.

Extensions in the homogenization model

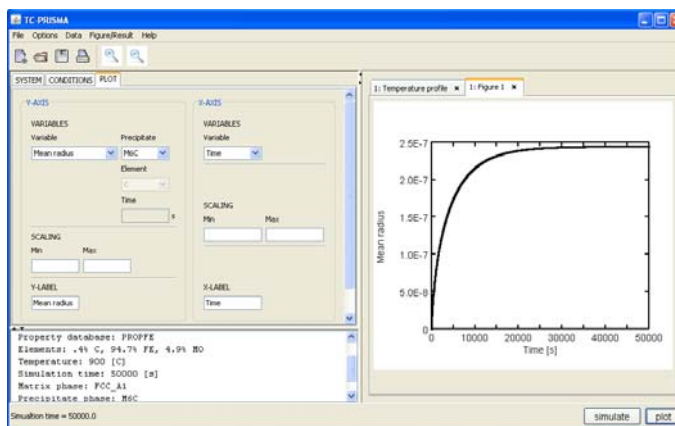
In the new version the homogenization model has been further improved and extended, e.g. new options for selecting homogenization functions have been added.

TC-PRISMA - software for precipitation kinetics

This is to inform that a new software tool (TC-PRISMA) for simulating precipitation kinetics in alloys is under development at Thermo-Calc Software.

TC-PRISMA is based on accurate models for nucleation, growth and coarsening, and when used in conjunction with accurately assessed thermodynamic, kinetic and property data (e.g. molar volumes, interfacial energies), it's a very powerful appropriate tool for predicting precipitation kinetics in alloy systems.

The figure on the right shows an example taken from the Graphical User Interface of TC-PRISMA that has been designed to be extremely easy to use. In the plot window a mean particle (M6C) radius can be seen plotted as function of time.



A first version of TC-PRISMA is scheduled for release during the end of 2008. In conjunction to this release a limited property database (containing e.g. interfacial energies) for steels will also be made available. However, it should be stressed already now that this type of property data is in general very difficult to determine and a property database of this kind will thus be somewhat approximate.

Database News

There are several new and updated databases available. Here we only have room to very briefly inform about the new updated version of TCFE. For more info related to this subject look at <http://www.thermocalc.com/Products/Databases.html> Please note that Databases are not covered by your software maintenance and support subscription, and updates needs to be purchase separately.

TCFE6 –TCS Steels/Fe-Alloys Database, version 6

In order to increase the predictive capability of this database, several significant re-assessments have been performed and incorporated in the updated version. The element Ca has been added and the alloying ranges for the elements C, Co, Cu, N, Ti and V have been extended.

The SIGMA phase is described with a new model in TCFE6 and new phases such as e.g. KAPPA, Z_PHASE and DIGENITE have been added. Several elements; B, Ca, Co, Cu, Mg, Nb, Si, V and Ti are now modelled to dissolve in additional phases such as LIQUID, FCC_A1, BCC_A2, different carbides, nitrides, sulphides and oxides. Major revisions regarding the solubility of Boron in LIQUID, FCC_A1, BCC_A2, HCP_A3, CEMENTITE, M23C6, M7C3, BN_HP4, CR2B_ORTH and M2B_TETR have been made.

Several oxide phases have been updated for the Fe-Al-Ca-Cr-Mg-Mn-Ni-Si-C-O system and a new model for the spinel and corundum phases has been implemented, which makes it possible to simulate diffusion inside these phases using the DICTRA software (also possible for other oxides such as halite) provided suitable mobility data are available.