



Thermo-Calc Software

No 32, September 2006

Editors: Anders Engström, Carl Lindqvist

Newsletter

Dear Thermo-Calc software user

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

Some unexpected and complex problems arose on the way, but the Thermo-Calc Software spirit would never give up development until we reached an accepted solution. Therefore, it has taken us longer than initially anticipated to complete the work, and this is something we feel sorry for and we have all ready started an action program to improve our development for the future and for our users.

Some of the new features now being introduced like, for example, the global minimization procedure are of a substantial nature and has required several iterations in order for us to get to a stage, where we feel that we have something of great benefit to our users.

The new versions will use the first level of global minimization during stepping and mapping and the work continues for the next level where our users have an option to make full use of the global minimization technique also during stepping and mapping. This important development and other work described in the following pages are part of our on-going strategy to offer the best and most stable products to our users. Even as this new release is being shipped, work has started on the next versions of the codes and it is our intention to ship the next releases within 12-18 months.

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 suggest that the new user's guides are consulted.

Best Regards

Dr Anders Engström
President, Thermo-Calc Software

*New releases from
Thermo-Calc Software*

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Common New Features:

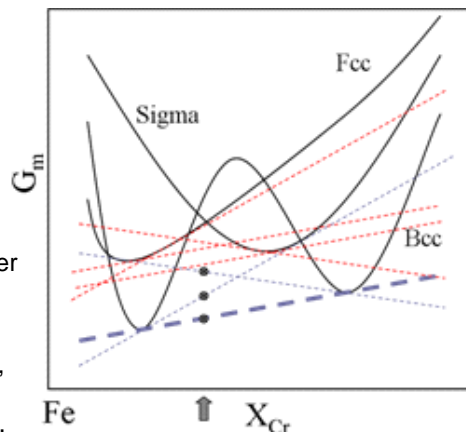
Thermo-Calc Classic ver. R & Thermo-Calc for Windows, TCW ver. 4

Global Minimization

A major improvement in the new version of Thermo-Calc is the implementation of a new global minimization routine, which ensures that truly stable phase equilibrium is calculated under various given conditions. In other words this will prevent that an undesired metastable or unstable equilibrium is calculated.

With this new technique, miscibility gaps can be automatically detected and additional composition sets will be created automatically. Therefore it will no longer be necessary for the user to specify these in advance.

At the moment fully supported conditions are conditions in N, n(), B, b(), w() and x(). For all other types of conditions a global test and corrections are performed until the lowest minimum is found.

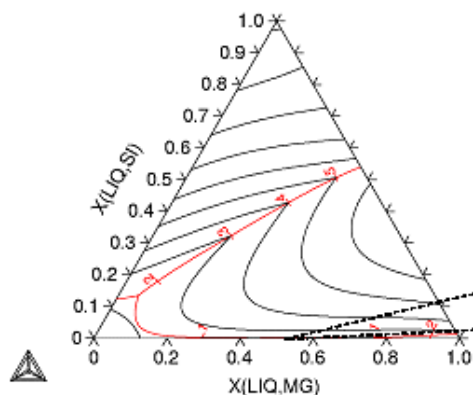


When stepping along a single axis and when mapping a diagram, a global minimization test will be performed during the initialization, but not later during the actual stepping and mapping. This strategy has been selected for the time being in order to keep computational times short, but a complete rewrite of the stepping/mapping is already ongoing and will be made available in the next release.

Automatic Calculation of Liquidus Surfaces

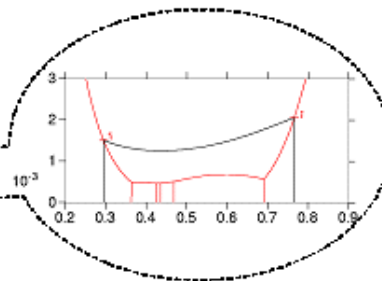
A module for calculating phase diagrams for ternary systems is introduced and allow for automatic calculation of 1) isothermal sections, 2) monovariant lines, and 3) projections of the liquidus surface. Plotted diagram for the latter type will include invariant, as well as isothermal lines. In addition, all the invariant reactions and their type are also identified and listed.

THERMO-CALC (2006.03.23:16.35) :AL-MG-SI (500C/1400C/100C) 18 s
 DATABASE:PTERN
 Z-AXIS = 400.0 + 100.0 * Z



INVARIANT REACTIONS:

- E 1: 557.88 C: LIQUID -> DIAMOND + FCC_A1 + MG2SI
- U 1: 451.54 C: LIQUID + AL12MG17 -> ALMG_DZE + MG2SI
- E 2: 449.84 C: LIQUID -> ALMG_BET + FCC_A1 + MG2SI
- U 2: 448.59 C: LIQUID + ALMG_DZE -> ALMG_UPS + MG2SI
- E 3: 448.09 C: LIQUID -> ALMG_BET + ALMG_UPS + MG2SI
- E 4: 436.38 C: LIQUID -> AL12MG17 + HCP_AS + MG2SI





Common New Features:

Thermo-Calc Classic ver. R & Thermo-Calc for Windows, TCW ver. 4

Scheil simulations

The equilibrium solidification result is now automatically superimposed (as a dashed line) with the non-equilibrium (Scheil) or partial-equilibrium (Scheil with back diffusion of interstitials) results on the same diagram without the need to calculate the equilibrium curve separately.

Graphic Output

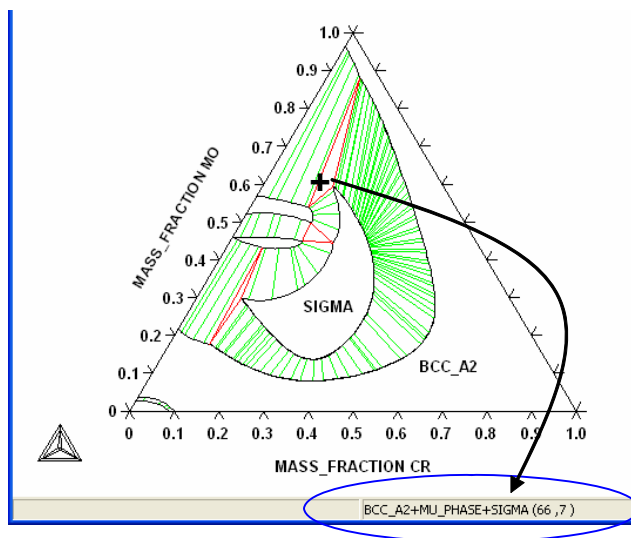
Plots can now be saved in an EMF format that is editable to some extent when opened in other software, such as Microsoft PowerPoint.

Post-processing

There is now a new feature to automatically detect (or identify) plotted lines in so-called “property diagrams”, i.e. diagrams created after stepping in one single variable. This is accomplished simply by placing the cursor near a line. The label of that particular line will then be displayed at the bottom of the graphical window.

In a similar fashion, by simply placing the cursor inside a region of a phase diagram, the stable phases in this phase field are automatically identified, see e.g. Fig. to the left.

It is now possible to directly export plotted diagram data into Microsoft Excel. At the moment this feature works only for so-called “property diagrams”, i.e. diagrams created after stepping in one single axis.





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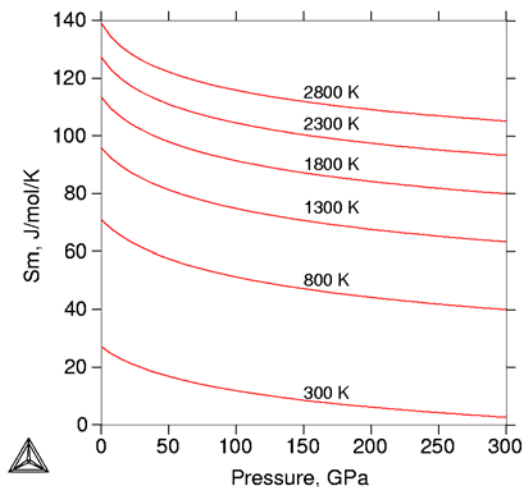
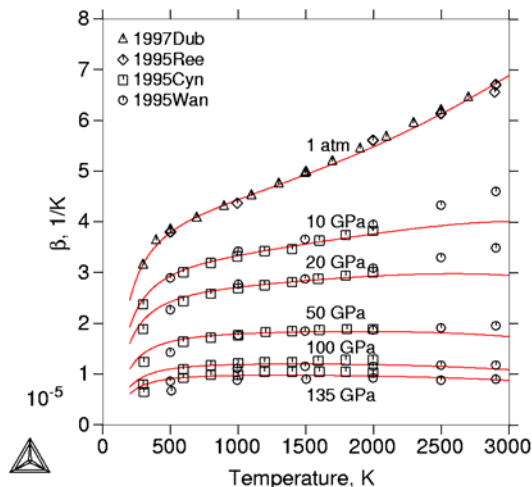
Newsletter

Common New Features:

Thermo-Calc Classic ver. R & Thermo-Calc for Windows, TCW ver. 4

Generalized PVT Model

In the previous and current version of Thermo-Calc, there are several thermodynamic models to handle pressure-volume-temperature EOS (equation of state) for metallic alloys and other varied forms of solids/minerals (carbides, nitrides, hydrides, oxides, sulfides, hydroxides, borides, phosphites, halites, silicates, carbonates, sulphates, nitrates, phosphates, etc.), as well as for liquids (melts/slag), aqueous solutions and gaseous mixtures. Specifically for alloys and minerals, the Murnaghan, Birch-Murnaghan and Modified Birch-Murnaghan models have been previously implemented in Thermo-Calc. Now a new model, called the Generalized PVT Model has been introduced, which compared to the aforementioned models does not produce anomalies at high T and P.



Furthermore, the new model allows for volume, thermal expansion, and bulk modulus at high T and high P to be modelled by using a simpler approach requiring less parameter. Details related to this new model will be published.

Do you use an older software version?

Have you terminated your Maintenance & Support Subscription?

Easy to solve!

Ask us, or your local sales representative for an upgrade to the latest version of your software.



Thermo-Calc Classic version R: Specific Changes

POLY Module

The price to pay for assuring a global minimum is an increase in computational time. That global minimization is used in a single equilibrium calculation will be the default, but it can of course be turned off by the user. This is accomplished by the command SET_MINIMIZATION_OPTIONS in the POLY-3 module. Furthermore, a regular minimization is performed if a minus sign is added after the command COMPUTE_EQUILIBRIUM, i.e. "COMPUTE_EQUILIBRIUM -", or "C_E -" etc.

POST Module

A new command in the POST, called LIST_DATA_TABLE, can be used for directly exporting plotted diagram data into Microsoft Excel. At the moment this feature works only for so-called "property diagrams", i.e. diagrams created after stepping along one single axis.

Another new feature has been included to quickly add a label with information on the stable phases inside a region in a plotted isothermal or isoplethal phase diagram, simply by "right-clicking the mouse" and select "add label" in the list displayed.

Plots can now be saved in EMF format, which is editable to some extent in other software, such as Microsoft PowerPoint. This is accomplished by using the SET_PLOT_FORMAT command and selecting device number 19 before plotting a diagram.

Using the command SET_PLOT_OPTION it is now possible under one of the options (PLOT SYMBOLS AT NODE POINTS) to indicate that one would like to visualise the actual points calculated in a diagram by plotting a symbol at each such node point.

Thermo-Calc for Windows version 4, TCW4: Specific Changes

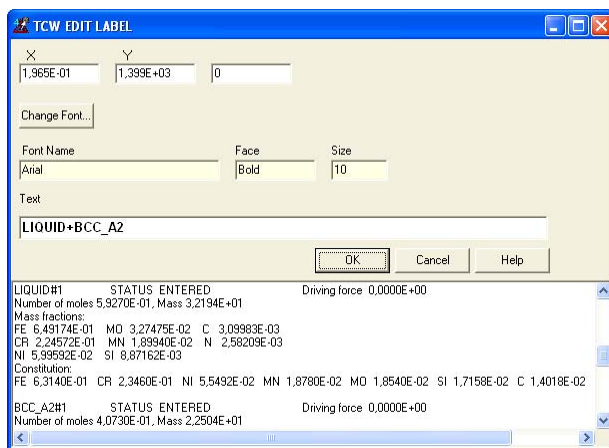
Graphical Output

An option has been added for including a raster in plotted diagrams.

It's now possible to directly open and plot .exp files. This is something several of our users have been asking for and it has now been added upon request.

It's now possible to "add labels" (with information about the stable phases inside a region) to plotted isothermal or isoplethal phase diagrams also by "right-clicking the mouse" and select "add label" in the action list displayed.

Information related to these labels can be viewed later and the actual label text can be edited and/or moved.





Thermo-Calc for Windows, TCW4: Specific Changes ... *Continued*

Combining Calculation Results

It's now possible to keep a calculation result, while e.g. repeating a calculation with slightly modified conditions and then to overlay the different results in the same diagram. This is accomplished by making sure the checkbox in the TCW Map/Step Definition Windows is unchecked when performing the second (and third etc.) calculation.

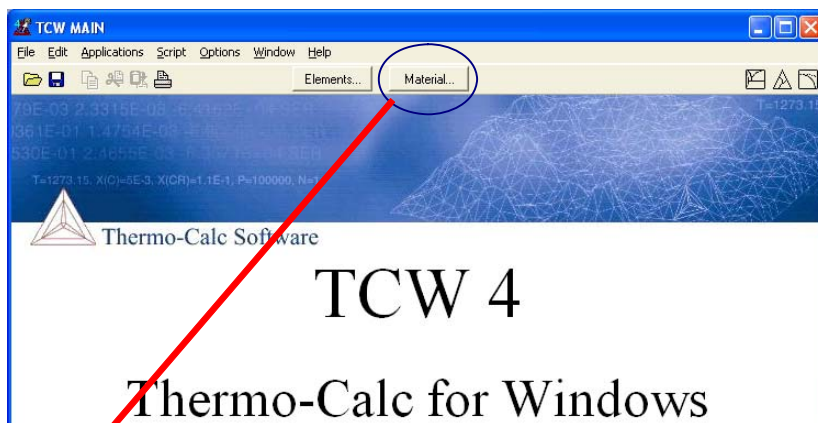
New Entry "Material"

This new entry allows the user to start certain type of calculations like;

- Single point equilibrium
- Single axis step
- Diagram mapping and Scheil),

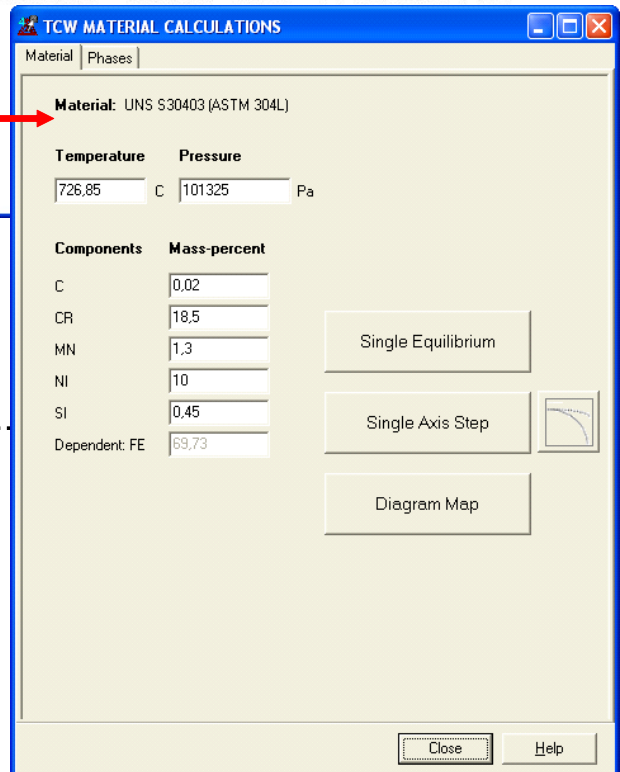
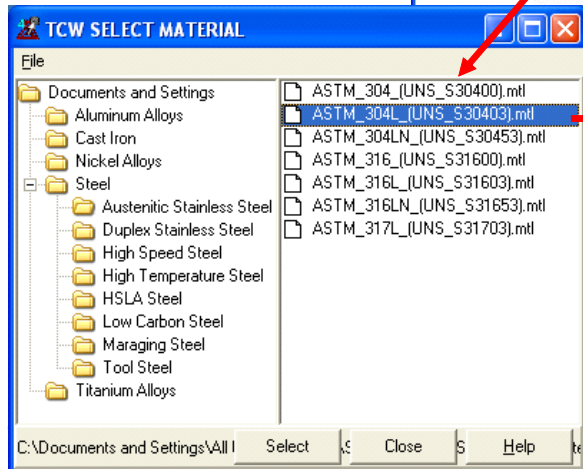
from predefined alloy compositions.

To perform calculations following this route will be easy and straight-forward.



TCW 4

Thermo-Calc for Windows



Alloy compositions can easily be added and modified according to the users own preferences.

It's also possible to access the predefined alloy compositions inside the "Elements" entry in order to perform other and more complex type of calculations starting from a specific alloy composition.



TC API version 4: New Functionalities

1st and 2nd derivatives of Gm

A new function named "tc_get_derivatives" has been introduced, which makes it possible to directly derive both first and second derivatives of Gm with respect to site-fractions.

Global minimization

By using the new command "tc_set_minimization_option" it's possible to specify that equilibrium calculations are performed using the global minimization technique recently introduced in Thermo-Calc. This will under most conditions ensure that a true global minimum is found. However, the price for this is an increase in the computational time.

TC MATLAB Toolbox version 4: New Functionalities

1st and 2nd derivatives of Gm

As for TC-API a new command named tc_get_derivatives has been introduced, which makes it possible to derive directly both first and second derivatives of Gm with respect to site-fractions.

Global minimization

As for TC-API there is a new command "tc_set_minimization", which allows for the user to specify that equilibrium calculations should when possible be performed using the global minimization technique recently introduced in Thermo-Calc.

TQ Interface version 6: New Functionalities

Thermodynamic and kinetic database handling

It is now possible from TQ-I to open and read data from a .TDB or .TDC file. This means that it is no longer necessary to first create a so-called .GES file by using Thermo-Calc Classic, and then read data from this file in TQ-I.

The new subroutines that support database handling work in a similar way to Thermo-Calc Classic, i.e. they can be used to:

- Open and append databases
- Define, reject, restore elements, species and phases
- Get data or reject system



TQ Interface version 6: New Functionalities ... *Continued*

Para-equilibrium calculation

A new subroutine for para-equilibrium calculation has been introduced. This subroutine can be used to obtain both the chemical driving force for nucleation and the equilibrium concentration under the para-equilibrium condition.

1st derivatives of Gm with respect to mole-fractions

A subroutine has been added for obtaining the first derivatives of Gm with respect to mole-fractions. This is helpful to users who are not familiar with the first derivative of Gm with respect to site-fractions, which can also be obtained in TQ-I since version 5.

2nd derivatives of Gm

A new subroutine has been introduced for calculating second derivatives of Gm with respect to site-fractions, i.e. the so-called thermodynamic factors.

Global minimization

If specified, equilibrium calculations can be performed using the global minimization technique recently introduced in Thermo-Calc. This will under most conditions ensure that a true global minimum is found. However, the price for this is an increase in the computational time.

DICTRA version 24: New Functionalities

Improved convergence

The main improvement in DICTRA version 24 is that an effort has been made in order to improve the convergence when the simulation involves moving phase boundaries, i.e. the algorithm that seeks a unique solution to this type of problem has been modified. It has also been found that for finding these solutions, varying a set of unknown activities is usually preferable to varying a set of unknown chemical potentials as has been the default. For that reason the default suggestion has now been changed to varying a set of unknown activities. However, specific calculations may still require that chemical potentials are varied. Furthermore, problems involving several cells require that chemical potentials are varied and hence for such problems the default suggestion remains unchanged.

Improvements in the PDE solver

Modifications to the Partial Differential Equation solver have resulted in improved numerical stability when solving the diffusion problem.

Improvements in the accounting

Multiple removal and addition of regions are now handled in a much more controlled manner.



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DICTRA version 24: New Functionalities ... Continued

New argument added to the SIMULATE-REACTION command

In order to avoid a simulation to stop and prompt for start-values every time a new region is created (i.e. a new phase appears), there is now a new argument "YES" to the "SIMULATE-REACTION" command. Invoking this argument will make the simulation continue by always using the default suggestions, i.e. it will have the same effect as hitting return several times when running interactively, or in a script file leaving several blank lines after the "SIMULATE-REACTION" command.

For version 25

For more than three years, we have been occupied by a major rewrite of the code in order to be able to handle diffusion also in "complex phases", in particular ionic phases (oxides). The modifications now being made will allow us to consider diffusion of not only the elements (e.g. Mn, Cr etc.) on a sub-lattice, but also the species (e.g. Mn, Mn²⁺, O²⁻, MnS etc.). Naturally, we had hoped to be able to include this new work already in version 24 of DICTRA, but this is unfortunately not the case. Instead this improvement is something we plan to include in version 25 of DICTRA.

Meet us and ask for a demonstration at:



44th
National
Metallurgists'
Day
13th to 16th
November
2006
Jamshedpur,
India

Training Courses

Check out our website for training courses.

Coming training courses are:

| | | |
|---------------------------|-------------------|------------------------|
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| Seminar | India, Hyderabad | 5 February, 2007 |
| Thermo-Calc Training | India, Hyderabad | 6-8 February, 2007 |
| Thermo-Calc & DICTRA | Australia | 20-21 March, 2007 |

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Until the next Thermo-Calc Software Newsletter, you are always most welcome to contact Thermo-Calc Software if you have any questions or comments regarding our products, services and partnership co-operation.

Contact details

General information:

info@thermocalc.se

Global Head Office:

Thermo-Calc Software
Stockholm Technology Park
Björnnäsvägen 21
SE-113 47 Stockholm
SWEDEN

E-mail: info@thermocalc.se
Office tel: +46 8 545 95930
Office fax: +46 8 673 3718

USA, Canada & Mexico:

Thermo-Calc Software, Inc
4160 Washington Road
McMurray
PA 15317
USA

E-mail: Paul@thermo-calc.com
Office tel: +1 724 731 0074
Office fax: +1 724 731 0078
Cell phone: +1 724 518 7334

Visit our website on the Internet, where you also can find much more information.

<http://www.thermocalc.com>

If you have specific needs and would like to discuss how Thermo-Calc Software can support you, please do not hesitate to contact us