Newsletter

Thermo-Calc Software

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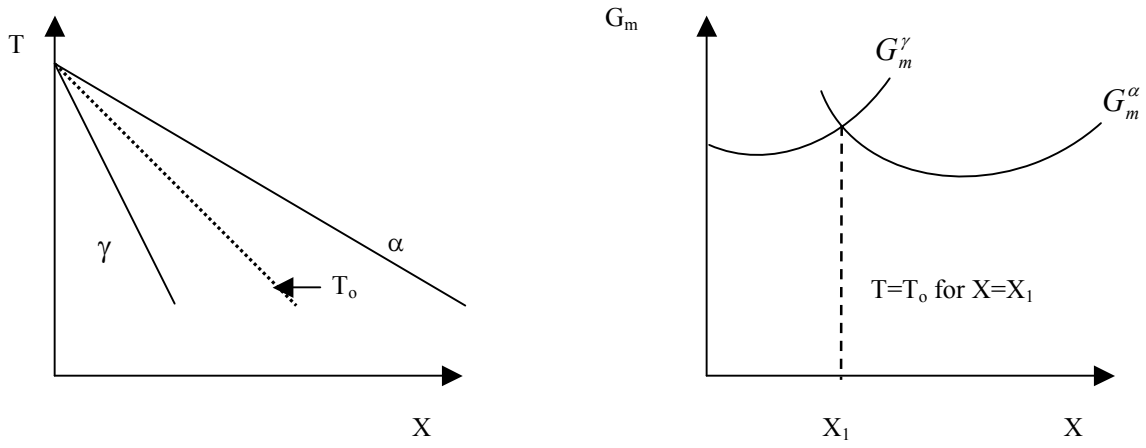
Thermo-Calc Classic, version P

Thermo-Calc Classic, version P is currently being tested for release. The new version contains a number of new features and the release will also include improved documentation and calculation examples. The new version is scheduled for release in November to all our maintenance customers.

Two of the major, new features in version P are the possibility to calculate T_0-temperatures and paraequilibrium. These features are described in more detail below.

T_0-temperature

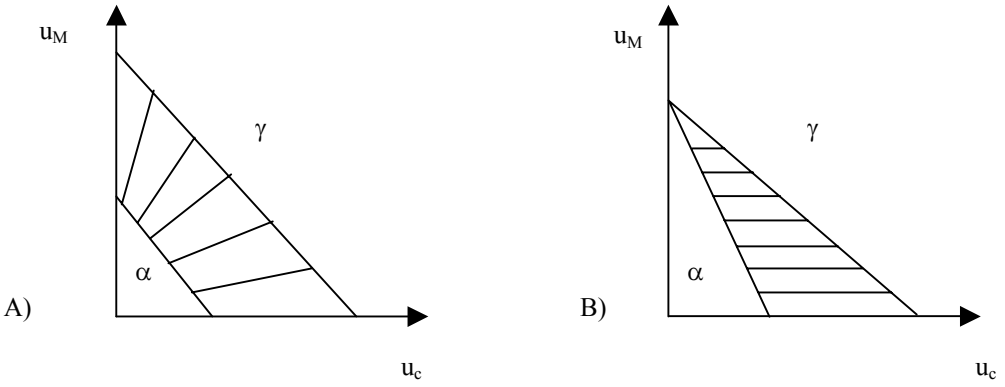
The T_0-temperature is defined as the temperature where two phases have the same Gibbs energy for a certain composition. The T_0-temperature is located within the two-phase field between the phases and it is the theoretical limit for a diffusionless transformation. Calculations of T_0-temperatures are thus of interest e.g. when studying diffusionless transformations. The principles for calculating the T_0-temperature is illustrated below



In version P of TCC a command for calculating the T_0-temperature has been implemented in the POLY3-module in the SPECIAL_OPTIONS command where one of the options now is T-ZERO TEMPERATURE. It has also been implemented as an option in the STEP command for calculations with one axis variable.

Paraequilibrium

Paraequilibrium conditions can occur when one component in an alloy can diffuse much faster than the others. Under these conditions it is possible to have a partly partitionless transformation where a new phase can form with different content of the mobile component but with the same composition of the slow diffusing components. Paraequilibrium can be calculated both in single equilibrium calculations and also in STEP calculations. Such calculations are useful e.g. when studying phase transformations in systems with large differences in the diffusivities of different elements. Transformations occurring under paraequilibrium conditions can be much more rapid than if full local equilibrium holds at the phase interface.



Ternary Fe-M-C diagram where M is a substitutional alloying element and C is the fast diffusing carbon. The composition variable u is defined as $\frac{x_i}{\sum_{j \in S} x_j}$ where the sum is taken for all substitutional alloying elements. Figure A shows the isothermal section and the two phase field $\alpha+\gamma$ for equilibrium conditions and figure B is the same isothermal section and two-phase field for paraequilibrium conditions.

Paraequilibrium calculations have been implemented in POLY3 in the SPECIAL_OPTIONS command where one of the options now is PARAEQUILIBRIUM. It has also been implemented as an option in the STEP command for calculations with one axis variable.

Other new features

Many other new features have been added into version P. The improvements in each module are listed below.

GES5

The maximum possible number of constituents in a non-ideal phase have been increased from 80 to 200.

PARROT

In PARROT it is now possible to store and restore the weights given to different experiments in an assessment. The commands STORE_ALL_WEIGHTS and RESTORE_ALL_WEIGHTS are used for this.

POLY3

The convergence for the COMPUTE_EQUILIBRIUM * command has been improved. Adding the * to the command employs a more robust technique for the equilibrium calculation.

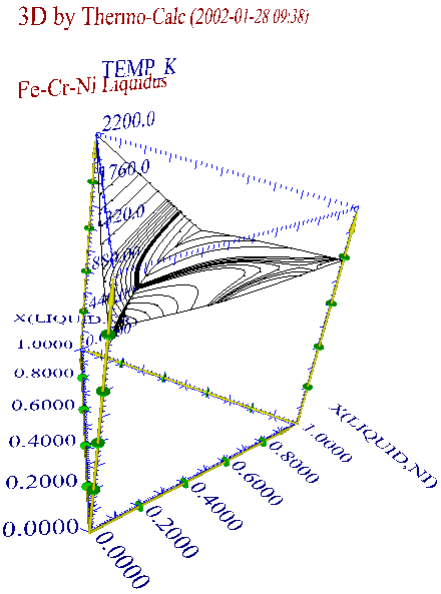
The COMPUTE_TRANSITION command has been improved. It is now possible to look for any new phase appearing when one condition is varied by using the keyword ANY instead of a phase name.

It is now possible to have a check of the internal stability of phases in POLY3. Using STABILITY_CHECK in the SPECIAL_OPTIONS command it is possible to check if any phase can be subject to spinodal decomposition.

POST

On the windows version of TCC there is a command DUMP_DIAGRAM that enables the user to convert the plotted diagrams to graphical formats (PNG,BMP,PDF,JPEG,TIFF), which are convenient to use in the Windows environment and in MS Office software.

Have you ever had problems when returning to a diagram plotted some time ago? Which conditions did I use? Which database? In version P the database and conditions used are automatically printed on the diagram.



TCC can now produce 3D plots! Routines for creating vrml-files (Virtual Reality Modelling Language) from plotted diagrams have been implemented in version P supporting triangular and tetrahedral diagrams. Vrml-files can be read, viewed and printed e.g. using one of the many plug-ins freely available for web browsers.

TDB

In the thermodynamic database module a new command SET_AUTO_APPEND has been implemented. This makes it possible to conveniently append a database with the same system definition.

Previously the database files for Unix systems and Pc/Windows have been incompatible due to different structures of the files. In version P a routine for converting database files has been implemented making it possible to read database files from both systems. The routine gives a warning message if conversion is necessary.

DICTRA version 22

A new version of Dictra, version 22, will be released in connection to the release of Thermo-Calc Classic version P. The new DICTRA release will contain e.g. models for diffusion in stoichiometric phases such as A_2B, incorporation of interfacial mobilities for moving phase boundaries and numerical integration/differentiation of plotted curves. This version of DICTRA will be presented in more detail in the next Newsletter.

Interface updates

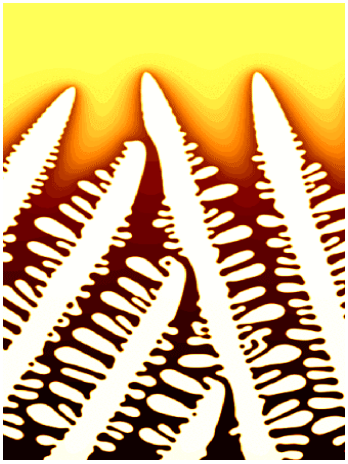
New versions of our programming interfaces based on the TC calculation engine version P are currently being developed. The interfaces

- TQ version 4 (includes the possibility to access kinetic data)
- TC-API interface, version P
- TC-Toolbox in MATLAB, version P

will soon be available.

If you are interested in more details about DICTRA_v22 or the programming interfaces, contact info@thermocalc.se.

MICRESS, phase field software with Thermo-Calc basis



MICRESS, a 2 and 3D phase-field software, is now being launched by our German partner ACCESS e.V. This software has been developed for simulation of microstructure evolution during phase transformations and especially the effect of different microstructures on the phase transformation kinetics can be investigated. Applications such as solidification, solid-state transformations, grain growth and recrystallisation can be studied.

MICRESS has been linked to Thermo-Calc using the latest version of the TQ interface (version 4). Using this version of the TQ interface, basically any thermodynamic or kinetic information as available in Thermo-Calc and/or DICTRA can be incorporated into your application software. The TQ interface provides MICRESS with a reliable basis for treating complex thermodynamic and kinetic behaviors in multicomponent alloys.

The Centre for Computational Thermodynamics

Thermo-Calc Software joins CCT

CCT is a joint research programme between **KTH, Department of Materials Science and Engineering** and the **Swedish Institute for Metals Research**, financed by the **Swedish Foundation for Strategic Research, SSF**, **Jernkontoret** and 12 Swedish companies. Thermo-Calc software is proud to be a member of this research program, which aims to create the best possible conditions for long-term fundamental research and for short-term applied industry-related research within the field of computational thermodynamics. The Programme director of CCT is Dr Malin Selleby from KTH.

The objective of the fundamental research is to develop new thermodynamic and kinetic models, and to make use of first principle calculations to be used in parallel with the classical CALPHAD technique of evaluation. Material production processes will be modelled using general thermodynamic information. The applied research will mainly focus on the development and update of thermodynamic databases. Thermodynamic databases for four groups of materials are being developed in close contact with industry, (1) cemented carbides, (2) stainless steels, (3) high speed steels/tool steels and (4) carbon steels/sintered steels.

New positions

President

Dr Anders Engström, who joined TCS last year in November has been appointed President of Thermo-Calc Software as of September 1, 2002.

Member of the Board

Dr Björn Uhrenius has been elected new member of the Board of Thermo-Calc Software. Björn Uhrenius is PhD from the Division of Physical Metallurgy at the Royal Inst of Technology in Stockholm. He has been Manager of R&D at Avesta Jernverks AB, Adjoined professor of Powder Metallurgy at KTH, Dept head of Powder Metallurgy at the Swedish Inst for Metals Research and now recently retired from a position as Vice President Research and Development at Sandvik Hard Materials.

Accounts

Mrs Danijela Aleksic has recently been employed to handle our accounts. Danijela will be responsible for all finance transactions including invoicing, payments etc.

Research & Development

Dr Muriel Mathon has recently been employed for projects involving Thermo-Calc and Dictra. She made her PhD in Thermochemistry in Marseille, France and has several years of experience from research as well as teaching.

Danijela Aleksic

Muriel Mathon

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