

Thermo-Calc Newsletter - Number 23, February, 1999

The 1998 year was a successful year for TCAB

We have been able to expand the market significantly, to release the new versions of Thermo-Calc (M), DICTRA (20), TC4A (2.0) and TQ Interface (2.0), to conduct and accomplish the development of some databases and software interfaces, and to improve our technical supporting facilities. We believe that such success will continue in the new year and future.

Distributions of New Versions of the Thermo-Calc and DICTRA Software

The Thermo-Calc Version M and DICTRA Version 20 have been distributed to our maintenance customers and new customers. With some delays due to a few later improvement and a new distribution framework, all such distributions should now be delivered.

The Thermo-Calc User's Guide is under updating right now. One can find all new examples for the version M in the installed TCEX area. A printed Thermo-Calc Examples Book will be sent out together the User's Guide which will be available in April.

The DICTRA User's Guide and Examples Book, both as PDF files, have been distributed together the DICTRA version 20 for all platforms (saved in the HELP area). We are also printing them on bonded books and will send them out to all our maintenance and new customers at the beginning of March. One can also view and browse these two PDF files from the Internet under <http://www.thermocalc.se/~dictra/examples.pdf>, and [~dictra/users_guide.pdf](http://www.thermocalc.se/~dictra/users_guide.pdf).

The Thermo-Calc version M new features were described in the previous issue of this Newsletter. For the PC Windows users, we will send out in April an extended version of executable files with a newly designed Thermo-Calc Graphic Window module which allows comprehensive graphic editing, automatic phase region identification, direct printing to any connected printer, copy and paste Thermo-Calc graphs into Microsoft Word or PowerPoint or other documents, and so on.

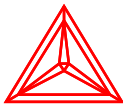
New TC and DICTRA Courses

Some TC and DICTRA courses are planned at KTH by TCAB, or will also be arranged by our agents or special partners, as listed below:

- Mar 17-19, 1999, TC Basic & Advanced Course (2+1 days) at KTH;
- Mar 22-24, 1999, DICTRA Course (3 days) at KTH;
- May, 1999, TC Course in Grenoble, France, arranged by Prof. I. Ansara (e-mail: iansara@ltpcm.inpg.fr)
- Oct 1999, TC Basic & Advanced Course (2+1 days) at KTH;
- Oct 1999, DICTRA Course (3 days) at KTH;
- Additionally, some TC and DICTRA courses will be arranged elsewhere by TCAB's local agents: Mr. Kiyoshi Hashimoto (fax: +81 3 5634 7338) in CRC Research Inst., Tokyo, Japan; Mr. Ron Shell (fax: +1 412 833 4580) in AEA Technology, Pittsburgh, USA;

For further information please visit our web site or contact us or the organizers directly.

Special Offers for Upgrading Thermo-Calc and DICTRA



To encourage our customers to have the software maintenance option and to use the software more extensively, TCAB has decided on giving special offers on various upgrades. For the upgrade from a Single-User to Site License and for an upgrade from an older version to the most current version, 20% of reduction based on the TCAB 1999' standard price lists can be obtained if a maintenance contract is signed at the same time.

These special offers are valid for the whole 1999 year and are applicable worldwide, but for the regions of North America (USA, Canada and Mexico) and Japan our agents have the rights to decide on the reduction margin. If you are interested in these special offers, please promptly contact with us or our agents.

Exploring the Applications of the TQ Interface

We highly encourage our customers to explore the applications of the TQ Interface (the third-party application programming interface which connects the powerful Thermo-Calc engine). TCAB will also launch some development projects on incorporating it with some renowned software packages which are widely used in many different applications.

The second version of the TQ Interface has been developed. A comprehensive TQ Interface User's Guide and Examples Book will be available in March. More examples applying the TQ Interface for various problems have been prepared.

The TQ Interface will be freely distributed to university customers for academic non-commercial uses.

TCAB as an Agent for Resales of ASM-APD Products

To provide our customers with more tools and services in R&D and dialy work related to materials science and engineering, TCAB has recently signed an agreement with ASM International, for marketing and sales of all kinds of ASM Alloy Phase Diagram products, ASM-published electronic products and ASM journals.

We welcome all of our existing and prospective customers (except from Japan) to contact with us for any purchase of such ASM-APD products.

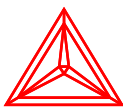
Some Other Connections

A combined TC/DICTRA Course (4 days, from Feb. 23rd to 26th) will be given at the Baoshan Steels, Ltd., in Shanghai, China, co-organized by Prof. Weijing Zhang at Univ. of Sci & Tech. Beijing and TCAB.

A series of lectures on Computational Thermodynamics and Thermo-Calc will be given between May 5 and 11 at Univ of Pittsburg, Carnegie Mellon Univ, MIT in Boston and Univ of Connecticut by Prof. Bo Sundman. Please contact Ron Shells or Larry Kaufman (lkaufman@juno.com) in Boston for details.

New Features of the DICTRA Version 20

The current release of DICTRA (version 20) mainly contains internal changes not visible for the ordinary users. This means that the default settings can be used in most cases and that less user interaction is needed in order to perform a successful simulation. Large parts of the program have been rewritten in order to make these improvements possible. A number of



"bugs" have been removed.

A summary of the major improvements and new features in the DICTRA version 20 is given below:

Modifications:

- Improved numerical stability: an alternative iteration procedure, using a different method, is used when the normal equation solver fails to find a solution.
- A new algorithm for finding starting values yields more robust simulations.
- In the modified output during the simulation, the amount of matter in the system is now normalized and presented as the average U-fractions in the system.
- A modified method to judge whether an interface has moved to far, is used when the flag CHECK-INTERFACE-POSITION is set.
- SET-SURFACE-TENSION now applies for the current cell, enabling for user to enter different functions for different cells.

New commands:

- The command SET-SIMULATION-CONDITIONS now has two additional options:

"USE FORCED STARTING VALUES IN EQUILIBRIUM CALCULATION" -
(where the default value is NO)

"ALWAYS CALCULATE STIFFNES MATRIX IN MULDIF" - (where the default value is YES)

The first option mainly concerns the calculation of the equilibrium when using the disperse model in DICTRA, where the equilibrium calculations sometimes fail due the abrupt changes in the composition over the region. The latter option determines how often the diffusion coefficient matrix is calculated when solving the partial differential equations (PDE) of a diffusion problem. The default setting is to calculate the diffusion coefficient matrix, yielding the stiffness matrix, at each iteration.

However, when setting this parameter to NO, it is only calculated at the first iteration and a constant stiffness matrix is used to obtain the solution to the PDEs. This will then lead to an implicit solution and therefore the degree of implicitity is automatically set to 1.

- The command SET-BOUNDARY-CONDITIONS GLOBAL now has an additional option: Q . This means that instead of controlling the temperature the amount of heat extracted from system per time unit is controlled. The amount of extracted heat per time unit is normalized and the size of the system is normalized to 1 mole of atoms.