

Thermo-Calc Newsletter - Number 18, April 1995

It is more than a year since the previous issue of this newsletter and I am sorry for this delay. But during 1994 I have been on leave from KTH and worked as a guest researcher at Max Planck Institute for metal research in Stuttgart. This have given contacts to new users and also many ideas for new features in Thermo-Calc.

Version K of Thermo-Calc

is now finished and the new features are described in this issue. A major improvement is the test for miscibility gaps which prevents many problems with metastable extrapolations during MAP and STEP.

Two new modules

One for binary phase diagrams and one for potential diagrams have been added. These use POLY-3 for their calculations but have simplified input. For the binary module it is necessary to have a special database with information about the binary diagrams. This will be provided with the SGTE databases. A special "mini-version" of Thermo-Calc with just the tabulation, binary and potential module is planned.

The new version of Thermo-Calc will be available on OS/2 as well as MS-DOS, all UNIX platforms and VAX/VMS. A Mac version may be released in the autumn. An update of the manual will also come later.

WWW or World Wide Web

Is a new facility to give information on Internet, the electronic network covering the whole world. You can find the latest information about KTH, our department and Thermo-calc or DICTRA, our software for diffusion simulations, on this network if you use "Mosaic", "Netscape" or any other net browsing software using the http: address above.

At Ringberg in the Bavarian alps

the work on a new solution database started in February 1995. At this workshop 40 eminent scientists from chemistry, metallurgy, geology and physics revised the models used for the pure elements and compounds, in particular their metastable extrapolations, using the most recent data and methodology. As the change of such "unary" data will require reassessment of all binary and higher order systems this will be the start of a completely new solution database. It is expected that a complete set of new "unary" data will be available at the end of this year.

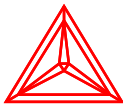
The workshop was arranged jointly by Max-Planck-Institute and KTH and sponsored by SGTE, the German research council, NIST and Calphad.

The cooperation with the Max-Planck-Institute

in Germany has also resulted in the three software programs for conversion between BINGSS and Thermo-Calc. A major effort has also gone into writing a book an assessments by Leo Lukas, Suzana Fries and Bo Sundman. This will be published after summer.

Cooperation with ThermoTech Ltd

in UK has resulted in a Windows program for PC, called ETTAN for phase fraction and phase composition plots using the STEP command in Thermo-Calc. ThermoTech Ltd also provides three Thermo-Calc compatible databases for Ti-alloys, Al-alloys and superalloys



(Ni-based).

Computational Thermodynamics has now been recognized as a scientific discipline as Bo Sundman has been appointed professor by KTH. The reason is of course the successful development of Thermo-Calc and the thermodynamic databases. However, new professors at KTH have to earn their own salary from external projects so the support from Thermo-Calc users is still needed to continue the work in the division.

New courses in Thermo-Calc will be given as follows:

- May 30 a seminar in Japan about Thermo-Calc, DICTRA and other software and databases. Please contact our agents, Kiyoshi Hashimoto, CRC Research Institute, tel 03 5634 5809 or fax 03 5634 7338 for more information.
- May 31-June 1 a Thermo-Calc course in Japan. Please contact CRC Research Institute for more information.
- June 12-13 a basic course at KTH
- June 14-15 an advanced course at KTH
- July 17-19 a basic+advanced course in Marseilles, France, in collaboration with Professor M Gaune-Escard, IUSTI. Please register by fax to 91 28 82 25.
- August 24-25 a basic course at KTH

The basic course requires that the user has some knowledge of thermodynamics and phase diagrams. The participants will have access to a PC or workstation to solve practical examples.

The advanced course requires familiarity with Thermo-Calc, at least of the level provided by the basic course. It will deal with assessments for extending the database, modelling of phases, the use of the reactor module and writing software to use Thermo-Calc in application packages.

The number of participants are limited, please use the enclosed form for application.

A new price list

will be valid from March 31 when version K will be released, including the new programs and databases. No new orders will be processed until this date. The price list will be sent on request. Unless you have a maintenance contract you must return the enclosed form to obtain the new version of Thermo-Calc.

The sales of software and databases during 1994 have increased a little compared to 1993. With the new modules Thermo-Calc should become an interesting alternative to software with less extensive facilities to handle non-ideal solution phases.