

### Thermo-Calc Newsletter - Number 19, November 1996

It has again been more than a year since the previous issue of this newsletter and I am sorry for this. During the last year several new persons have started in the group and some have left. A short presentation of all in the division of Computational Thermodynamics can be found on the web site above, <http://www.met.kth.se/tc>.

#### **Version L of Thermo-Calc**

is now finished and the new features are described in this issue. This year two more modules have been added, one for Scheil solidification simulation and one for Pourbaix diagram calculations.

The new version of Thermo-Calc will be available on DOS, Windows-95, Windows-NT, and all UNIX platforms we know about, including LINUX for PC. The Mac version is still in the pipe-line and seems to prefer to stay there. All the manuals have also been updated and converted to LaTeX and are available on the net. The WWW server with the web page for Thermo-Calc or DICTRA, our software for diffusion simulations, is given above.

#### **TQ as a subroutine package**

has been requested a number of times and such a package has been under development during the last years. It is now available for testing and will be delivered free with the new version L to all UNIX platforms. For PC it will be delivered upon request (it requires an extra floppy) and it will require the Microsoft Fortran package. This package has a standardized interface developed in an EU Science project together with LTH in Aachen and HTK in Helsinki. It should be possible to use the TQ or the ChemApp package without changing your source code.

#### **The use of thermodynamic calculations**

for a number of different applications is described in a recent book, the SGTE casebook. This is published by the Institute of Materials, UK and has contributions from all members of SGTE. One copy will be delivered free to those who have a maintenance contract for Thermo-Calc.

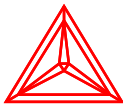
#### **The billing for Thermo-Calc**

will soon be made by an independent accounting company rather than through the Royal Institute. We hope our customers will be satisfied with this service which will make it possible to use more of the income for grants and projects to support the development of Thermo-Calc and the databases.

Revision of old licenses will be made in connection with updates of the software. All who have an old license on behalf of the department of Physical Metallurgy will have to sign a new contract with the Foundation before we can provide an update. Those who still continue to use an old version of Thermo-Calc are not affected by this. There will be no charge for this revision.

#### **The DICTRA system**

for simulation of diffusion controlled phase transformations is now spreading. This has led to a number of new TC customers also, as DICTRA requires TC as thermodynamic package. DICTRA make use of the unique feature in Thermo-Calc that TC can provide analytical values of all second derivatives of the Gibbs energy for each phase with respect to all its



fraction variables, temperature and pressure. These are needed to calculate the thermodynamic factor in the diffusion matrix. No other thermodynamic subroutine package is known to have this feature.

### **At Ringberg, in the Bavarian alps**

a second workshop was arranged in March 1996. This dealt with models for solution phases and covered topics like liquids, ordered phases, phases with order/disorder transformations, semiconductors and oxide phases. At the workshop 40 scientists from chemistry, metallurgy, geology and physics discussed in small groups and presented results in lectures. The proceedings from this workshop is planned to appear in the Calphad Journal. The workshop was arranged jointly by Max-Planck-Institute and KTH and sponsored by SGTE, the German research council, NIST and Calphad.

### **Cooperation with ThermoTech Ltd**

in UK has resulted in an update of the TC-Fe database. This is described more later. There will also be a new release of ETTAN including a Scheil simulation option.

### **New courses in Thermo-Calc will be arranged as follows:**

- Dec 9-10 in Gothenburg. This course is fully subscribed already.
- Jan 8-10 (preliminary) a combined basic and advanced course at KTH.
- May 15-16 (preliminary) in USA in connection with the Calphad meeting.

The basic course requires that the user has some knowledge of thermodynamics and phase diagrams. 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 is limited, please use the enclosed form for application.

### **A new price list**

will be valid from December when version L is released, including the new programs and databases. The price list will be sent on request. All with a maintenance contract will receive the new version automatically, but if you have no maintenance or want to make changes or additions you must return the enclosed form to obtain the new version of Thermo-Calc.

The sales of software and databases during 1995 and 1996 have increased considerably compared to 1994. With the new modules Thermo-Calc should become an interesting alternative to software with less extensive facilities to handle non-ideal solution phases.