Thermo-Calc Software

# Computational Thermodynamics on the move!

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The news of the first six month of 2009 have included words such as crisis, reduction, loss etc.. Despite the negative trends in global economy, we in Thermo-Calc Software do our best to keep an optimistic approach and a long term focus. Therefore we are happy and proud of the distributed new software versions, Thermo-Calc versions S & 5 and DICTRA 25, which saw daylight in the middle of the recession. The realisation of this long term, and sometimes really difficult, development work concerning these new software versions, as well as turning it into the useful tool you demand from us, have been a tough but stimulating challenge for us to overcome. A challenge that for periods has involved most everyone in the Thermo-Calc Software company. As a part of this new release, we have also implemented a new licensing system that we believe will be an improvement for both you and us in the long run. However, we have been forced to solve some problems by getting in to the very details in areas which was new to both us and our users IT departments. This sometimes required more of our time than expected, which unfortunately resulted in situations where some of our users had to wait for help which we deeply apologize and are truly sorry for. On the positive side, the late release was also a proof of that our improved quality assurance systems worked well and the new testing methods we have introduced is matching our ambition to supply the best tool in computational thermodynamics.

We now hope that all of our maintenance and support subscribers around the world have installed and started using the new versions and that you show interest in the NEW Database versions on page 2 in this issue.

In our optimistic approach, we must also asks the question if the recession can initiate more research and development? We do hope that the negative down-turn in production can give more new ideas and more research and development. We also would like to use this opportunity to welcome all new users of Thermo-Calc and DICTRA.

Yours Sincerely Carl Lindqvist, President

## "Congratulations"

Thermo-Calc Software staff celebrated the Swedish Midsummer in June with a traditional pic-nic in the nearby park close to our office. The pic-nic included an extraordinary interesting game of "Kubb", resulting in a total loss for "Team Dynamic" against the new champions "Team Kinetic". Both teams have now joined forces again to meet the daily challenges, but a new game will be held next summer. Anyone can easily make and learn how to play. *More info about the game: http://en.wikipedia.org/wiki/Kubb* 



July 2009

Summer celebration by the winning TCSAB "Team Kinetic" .

## <u>NEW DATABASES</u>

In July 2009, there are 5 new database versions released that can bring new insight and understanding of thermodynamic and kinetic problems.

• ION3: TCS Ionic Solutions Database

The elements Mn, Y and Zr have been added and the number of phases has increased to 282. A new model for the spinel and corundum phases has been implemented which makes it possible to simulate diffusion inside these phases using the DICTRA software (also possible for other oxides such as halite) provided suitable mobility data are available.

- STBC2: SGTE Thermal barrier coatings database The current version, STBC2, is the second version commercially released as a standard Thermo-Calc/SGTE application database. The database chemical framework remain for the ZrO2-Gd2O3-Y2O3-Al2O3 system, but contain re-assessed data for the ZrO2-Gd2O3 and Gd2O3-Al2O3. Data has also been re-assessed for ternary system for consistencies of tie-lines with experimental data.
- TTAL7: Thermotech Al-based Alloys Database New Element: Li
- TTNI8: Thermotech Ni-based Superalloys Database: New element: Pt
- MOBFE: TCS Steels/Fe-Alloys Mobility Database
   MOBFE1 is a kinetic database containing mobility data limited to Fe-based alloys. Data
  is present in a format suitable for simulation of diffusion controlled phenomena using the
  DICTRA simulation software, and/or for use together with any Thermo-Calc programming interface. MOBFE1 is compatible and recommended for use in combination with
  the TCFE6 (TCS Steels/Fe-Alloys Database) thermodynamic database. The MOB2 database is intended for use with TCFE5 and older versions as well as with SSOL.

To upgrade from older versions you just have to contact your local sales representative or contact us by sending an e-mail to info@thermocalc.se.

Learn more about the improvements and the new database versions by checking our website where you find detailed database descriptions can be found on **www.thermocalc.com**.

You are also most welcome to contact us any time if you have any questions or just have requests that lays outside the scope of any commercial database available today.

> Did you know, that you can get the database information by pressing F2 with the cursor in the database field in Thermo-Calc for Windows?

## <u>TCS Support</u>

You can now help us to help you to get quicker support by supplying to your e-mail the following information:

- 1) Your site number. You find the site number on your license file, invoices etc.
- 2) Computer information by running the support tool "*Diagnostics tool*" available for free on the support page on our website. When the files are extracted a folder tclog will be created with the files in it. Run the file tclog.bat by double-clicking on it. If any error messages occure, just click OK and go on. This will create a text file tclog.log. Send this file to support@thermocalc.se together with a description of your problem.
- 3) Complete contact information for you.

The support office at Thermo-Calc Software handle incoming issues one by one and as quick as ever possible.

Do you regularly check our website for new patches ?

# <u>MEET US</u>

You can meet representatives from Thermo-Calc Software to see live demonstrations of the software and discuss how the software can support your specific needs at the following occasions:

- SIMAT, Beijing, China 23-27 August 2009
- Heat Treat, Indianapolis, USA, 14-17 September 2009
- MODERN PROBLEMS OF PHYSICAL METALLURGY OF NON-FERROUS AL-LOYS, MISIS, MOSCOW, Russia, 1-2 October 2009
- Computational Thermodynamics in Materials Research and Development Applications, Seoul, Korea, October 9 2009.
- MS&T09, Pittsburgh, USA, 26-29 October 2009

# TRAINING COURSES

Do you, or anyone you know, need to become more skilled in the use of the software? We have now scheduled the following training courses during 2009 for Thermo-Calc and DICTRA:

#### Autumn 2009

- Thermo-Calc Training in Aachen, Germany 8-11 September 2009
- Thermo-Calc Classic Training Course (2 Days), Oct 15-16 2009
- Thermo-Calc Windows Training Course (2 Days), Oct 15-16 2009
- DICTRA Training Course (3 days), Oct 19-21 2009

For more information about the course, accommodation etc. please chck our website or contact us by sending an e-mail to ake@thermocalc.se.



Did you know? We can arrange tailor-made training courses for your site.

## <u>Thermo-Calc Courses</u>

## Basic Thermo-Calc for Windows training course in Stockholm

This is the course where you learn how optimise your use of the user friendly interface. The course includes calculations of phase equilibria, property diagrams and phase diagrams. You will also calculate other diagrams such as isothermal, isoplethal sections and learn how to run solidification simulations by using the scheil module.

#### Advanced Thermo-Calc for Windows training course in Stockholm

The course cover among others, how to enter and use your own functions with the software for more advanced and application related problems and much more.

### Basic Thermo-Calc Classic training course in Stockholm

The basic course include calculation of phase equilibria, property diagrams and phase diagrams of alloys using Thermo-Calc Classic. Different types of phase diagrams such as isothermal and isoplethal sections are also calculated, and much more.

#### Thermo-Calc Advanced course in Stockholm

The advanced course contains calculations including user-defined functions, liquidus surfaces. Calculation involving other types of systems such as oxides or gases are also performed. Thermodynamic databases and the use of programming interfaces are discussed. This course is a continuation of Thermo-Calc Classic Basic course.

## **DICTRA Training Course**

## **DICTRA** course

A course for new and experienced DICTRA users that teaches you how to perform different kinds of diffusion simulations using DICTRA. Multicomponent diffusion theory and the creation of mobility databases are also discussed in the course. Some prior knowledge of Thermo-Calc is an advantage but not a requirement to attend this course.



Hands on teaching

## <u>NEW Faces within Thermo-Calc</u>

Once again we are happy to greet our two new colleagues, Samuel Hallström and Johan Jeppsson.

*Samuel* did his Ph.D studies at KTH, where he worked with thermodynamic modeling of high temperature nickel base alloys, and modeling and simulation of diffusion in oxide systems. Other interests are mostly related to family, computers, and physical exercise.

*Johan* did his PhD studies at KTH with the main emphasis on development of microstructure models for precipitation reactions in structural materials, grain growth in cemented carbides and one phase materials.



Samuel and Johan bringing in fresh ideas and clean up old technologies such as the floppy discs of the past above. Do you remember the packs of floppy

More information available at www.thermocalc.com