

# Thermo-Calc Software

**Newsletter**



**No 33, June 2007**  
Editors: Anders Engström, Carl Lindqvist

## Dear Thermo-Calc User

It's really amazing how quickly time can pass when you are enjoying what you are doing. It seems like yesterday, but in reality 10 years have now passed since the company Thermo-Calc Software AB was registered. The company was created in 1997 by researchers from the Royal Institute of Technology in Stockholm, Sweden, who had been involved in developing the software for about two decades. All involved researchers had at this time already donated their individual rights connected to the software to a non-profit foundation, and this foundation became and still is the majority owner of the company Thermo-Calc Software AB. The purpose with establishing a company was to manage sales and support of Thermo-Calc, DICTRA and their associated databases.

Dr. Pingfang Shi was the very first employee in the company and for a couple of months he was alone in the company before some additional staff could be recruited. The company has since the start had a steady growth and today keeps 16 employees, and additionally have a large network of local representatives, partners and associates. This development would not have been possible without all our fantastic supporters all over the world. We would really like to take this opportunity to thank all of you for your contributions. In order to honour this 10 year anniversary there will be a seminar in Stockholm on October 18-19th, 2007. Several distinguished speakers will take part and you are all more than welcome to join us. More information on this will follow.

One may wonder what another 10 years will bring into the field of computational thermodynamics. It's not easy to predict, but we can be reasonably sure that computer speeds will continue to increase, and continue to open up new possibilities in our field. Approximately half of the employees in Thermo-Calc Software AB are today dedicated to development, i.e. to improve existing software, databases, as well as to develop completely new products in order to meet the future needs from our clients. Well, let me conclude by stating that we for sure are looking forward to the next 10 years with great confidence. Oh, and by the way, Dr. Pingfang Shi is still working in the company.

Best Regards,  
Dr Anders Engström  
President, Thermo-Calc Software



Thermo-Calc Software celebrates its 10 years anniversary as a company with a 2 days seminar 18 and 19 of October in Stockholm. We welcome all our customers and partners to attend this seminar. Please confirm your interest by sending an e-mail to us.

## Future methods for designing industrial materials

Thermo-Calc Software is a member of a new scientific research centre at the Royal Institute of Technology in Stockholm, Sweden. The new centre for hierarchic design of industrial materials, HERO-M will focus on development of new methods for designing materials for industrial applications. The methods shall explain structural changes and transformation during manufacturing, heat treatment and use of materials.



## Software Updates

Software updates for Thermo-Calc Classic ver. R (TCCR), Thermo-Calc for Windows ver. 4 (TCW4), and DICTRA ver. 24 have been made available for download from our website from the end of June 2007 at: [http://www.thermocalc.se/DOWNLOAD\\_AREA/Updates.html](http://www.thermocalc.se/DOWNLOAD_AREA/Updates.html)

Below is a summary of the improvements in the updates.

### Thermo-Calc (both Thermo-Calc for Windows and Classic)

The post-processor in Scheil module has been almost completely rewritten. The reason for this is to make it possible to also plot:

- Total heat evolution. Note that previously only the latent heat evolution (i.e. the heat released as a result of the phase transformation itself) was calculated.
- Apparent Cp.

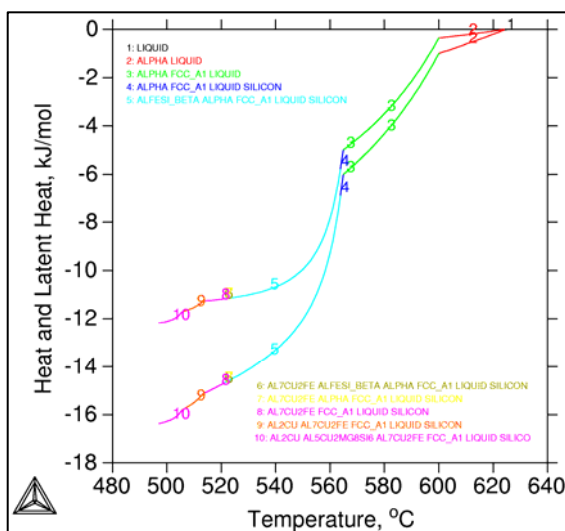


Fig. 1: Calculated total heat and latent heat for an Al-alloy.

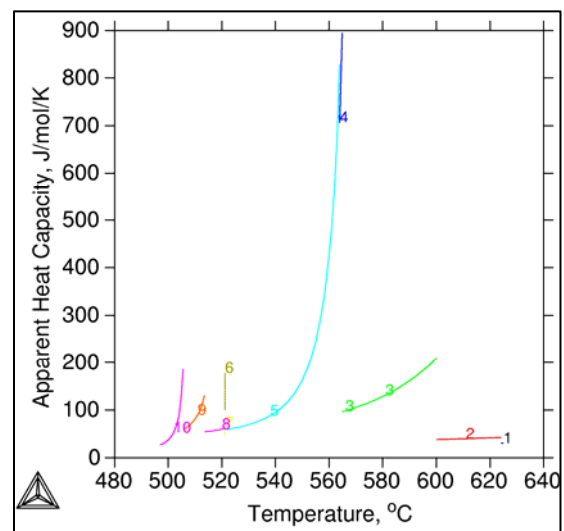


Fig. 2: Calculated apparent heat capacity for the same Al-alloy as in Fig. 1

The Scheil module has also been modified in order to make it possible to use the volume data now present in some databases, such as e.g. TCFE5.

When performing a simulation using TCFE5 it's now possible to calculate and plot also:

- Volume for a phase or the whole system
- Density for a phase or the whole system
- Apparent thermal expansion

In addition, the problem of ugly "breaks or gaps" appearing in some earlier Scheil plots has been solved.

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## Software Updates *continued*

DICTRA

Some minor improvements and bug fixes can be reported, e.g.

- Some improvement introduced in reading/writing of macro, experimental and store files.
- Bug introduced for ver. 24 in the dispersed diffusion model has been corrected.
- Diffusion model updated in order to handle cases where an element is present as an interstitial in one phase and as a substitution in another.

In addition, a new model for solving problems involving diffusion through a multiphase mixture (Beta version) has been introduced, see the new example exd3.

## Tip from Support: Adding new databases version to Thermo-Calc for Windows

When you order databases upgrades, it is recommended that you do not forget to also update your materials files for Thermo-Calc for Windows, where the database is used. The materials files can be edited either from Thermo-Calc for Windows or by accessing the files from the folder where you keep these. The path to the directory is set in the options menu.

## Metallurgists meeting Thermo-Calc at NMD 2006

The annual event National Metallurgist Day in Jamshedpur, India was hosted by Tata Steel. In combination with the conferences, we had the honour to meet some of the best metallurgists and material scientists in India, and also from other parts of the world. The visitors could attend on site demonstrations of the new software versions. It was also a great pleasure for us to meet users and friends.

*Carl and Mr Babburi ready for the NMD visitors.*



Magnus Ekbäck (left), R&D Director, Sandvik Coromant  
Johan Bratberg (right), Thermo-Calc Software

## New prize winning face

In November 2006, we could welcome Dr. Johan Bratberg to join Thermo-Calc Software AB.

In March 2007, Johan won the most honourable Sandvik Coromant Materials Award 2007 for his research work concerning complex carbide systems. The knowledge of the carbide systems is an important part in for example development and engineering of tool steels, high speed steels and hard materials.

Apart from winning awards and being an important part of the company, Johan is very fond of fishing and travelling.

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## New Database Versions

New database versions of the SGTE Substance Database (SSUB) and the SGTE Solutions Database (SSOL4) have been released. More technical information will be posted on our website shortly.

## New Partner in China

We are honoured to welcome Su Hang, Wang Zhuo, Chai Feng and colleagues at the China Iron and Steel research Institute Group as new Thermo-Calc Software Agent in China.

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## New Book: Computational Thermodynamics, The Calphad Method



Phase diagrams are used in materials research and engineering to understand the interrelationship between composition, microstructure and process conditions. In complex systems, computational methods such as CALPHAD (calculation of phase diagrams), are employed to calculate the thermodynamic properties and simulate multicomponent phase behaviour. Written by recognized experts in the field, this is the first introductory guide to the CALPHAD method, providing a theoretical and practical approach. Building on core thermodynamic principles, this book applies crystallography, first principles methods and experimental data to model the thermodynamic properties for each phase using the CALPHAD method. With a chapter dedicated to creating thermodynamic databases, the reader will be confident in assessing, optimizing and validating complex thermodynamic systems alongside database construction and management. Several case studies put the methods into a practical context making this suitable for use on advanced materials design and engineering courses and an invaluable reference to those using thermodynamic data in their research or in practical applications.

Contact: <http://www.cambridge.org/9780521868112>

You find much more information on our website

<http://www.thermocalc.com>