



Thermo-Calc Software

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During the end of last year and the beginning of 2003 we at Thermo-Calc Software have been busy distributing the new releases of our software to all our customers having a Maintenance & Support subscription. Already, we have had a number of positive reactions concerning improvements made, and the new functionality introduced in TCC version P, DICTRA version 22, and in particular concerning TCW version 2.1. We also had some problem reports. We appreciate this type of feedback, which is very helpful for us in our work to improve the software. Most of the problems have been already dealt with and you may find patches for download on our homepage (www.thermocalc.com/download/updates.html). We recommend our customers to regularly visit our homepage and check for the latest updates. Simply download these patches and replace your existing executable.

Some customers have been concerned about the encryption of databases, and more specifically about the fact that for some of our databases (TCFE, TCNI, ION, SLAG, TCPM, TCES and MOB) it is not possible to list any of the parameters inside the database. Due to customers reactions, we have decided to provide customer that have a strong need to see the parameters inside the database the possibility to do so, after signing a database license agreement. Please contact us if you require this option. The SGTE databases (SSOL and SSUB) are also encrypted, but please note that all parameters inside the databases can already now be listed if you are using TCC.

During the remains of this year we will be focusing on the development of the next releases of our software, e.g. TCC version Q, TCW version 3 and DICTRA version 23. Our ambition is to release these coming versions in about one year's time. As always, we are interested in having your comments and suggestions on how to improve our software. Please feel free to provide us with your ideas through feedback@thermocalc.se.

New Demo versions available

Demo versions of our software for PC/Windows may be downloaded from our homepage. Current demo versions are TCC version P and TCW version 2.1. The demo versions are restricted in that sense that it is possible only to perform calculations by defining less than 4 elements. Besides this restriction all the functionality of the software is included.

Download latest patches

Patches (the latest updated versions of a software or interface) that include smaller improvements, bug-fixes, made after the release of the new version, may also be downloaded from our homepage. With a valid license for the corresponding version of a specific software/interface, you can download such a patch, and substitute the corresponding old binary file with the downloaded one. We encourage all users to regularly check for new updates on www.thermocalc.com/download/updates.html.

DICTRA version 22

The most important improvement in version 22 is certainly the possibility to model diffusion in stoichiometric phases without any freedom, such as A2B. This will open up for several new applications to be treated, e.g. bonding of dissimilar materials where intermetallic phases are formed. At the moment, there is a limitation due to the fact that the available kinetic databases do not yet contain much mobility data for such phases. However, work is already in progress to generate such data, and in the meantime the advanced user can always enter such data himself. The procedure and syntaxes for adding such data is the same as for an ordinary solution phase.

Another important improvement is the possibility to simulate interfacial mobility controlled phase transformations. This is achieved by adding a Gibbs-energy contribution to the growing phase. Such an example has been included in the new DICTRA version 22 Examples Book, see ex. b6.

In some extreme cases, i.e. when treating problems with more than 150 grid points and having more than 10 diffusing species, the workspace inside DICTRA has not been large enough. This workspace has now been increased and it is possible to treat these large systems, i.e. simulations can now be performed with >10 elements and having several (>200) grid points.

There is now also a possibility to numerically integrate and differentiate plotted curves in the POST processor. The commands for this are simply "INTEGRATE_VALUES" and "DIFFERENTIATE_VALUES". It should be noted however that it is up to the user to set the correct scaling after using these commands.

Updated and New Databases

Several updated and new Thermo-Calc and DICTRA databases are introduced to our customers, as briefly described below. For more details of using such databases, please refer to the Database Description Forms documented in the Thermo-Calc and DICTRA Users Guides and our web site, or please contact us at info@thermocalc.se.

Updated Databases

TCFE3: TCS Steels/Fe-Alloys Database, V3.0 (2002)

On the basis of TCFE2 (i.e., TCFE2K or TC-FE2000 of 1999), further implementations have been made on:

- Improved data for the important sigma phase in stainless steels;
- Addition of data for the binary Nb-Ni system;
- Improved data for the ternary Fe-Cr-Mo system;
- Improved data for the ternary Cr-Mo-Ni system;
- Improved data for the fcc Ti(C,N) carbonitride;
- Some minor improvements for other systems.

One of the major improvements is the greatly improved ability for predicting the important sigma-phase in stainless steels. *Figure 1* shows a comparison among calculated results using the TCFE3, TCFE2 and SSOL databases for a duplex stainless steel.

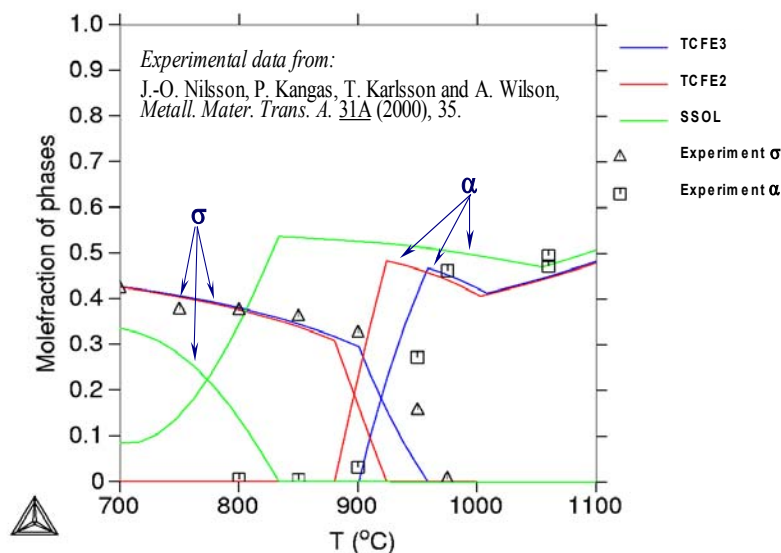


Figure 1. Calculated and experimental equilibrium phase fractions of ferrite and sigma-phase for a duplex stainless steel as a function of temperature. The calculations were performed with three different thermodynamic databases, TCFE3, TCFE2 and SSOL. The experimental data were taken from Nilsson *et al.* (2000).

It is recommended to upgrade from earlier versions of steels databases [e.g., TCFE1 (or the so-called TCFE_subset or TC_Alloy) of 1992, FEDATA of 1996, and TCFE2 of 1999] to TCFE3. Special discount offers are now available for the upgrades from TCFE2 and FEDATA.

Other updated databases:

As listed in *Table 1*, there are some other Thermo-Calc and DICTRA databases that have been recently updated and have been made commercially available for upgrades and new purchases.

Table 1. Some other updated Thermo-Calc and DICTRA databases

<i>Name & Version (Date)</i>	<i>Major Improvements and Options for Upgrades</i>
SSUB3 SGTE Substances Database V3.0 (2001, with some minor modifications made in April 2002)	Based on SSUB2 (of 1998), it now contains assessed thermochemical data for about 5000 (extended from about 4000 in SSUB2) condensed compounds or gaseous species within a chemical framework of 101 elements (which are the same as in PURE4, <i>i.e.</i> , with 16 additional elements and 2 hydrogen isotopes). <u>Upgrade:</u> from SSUB1/2 (free for all SSUB users with TCC/TCW maintenance).
SLAG2 TC Slag Fe-containing Database V2.0 (2002)	Based on SLAG1 (of 1992, with minor modification made in 1998), it contains improved thermodynamic data for liquid slag (covering 12 elements Al-Ca-Cr-Fe-Mg-Mn-Na-Si-O-S-P-F), Fe-rich liquid (including 26 dilute components Ag-Al-B-C-Ca-Co-Cr-Cu-H-Mg-Mn-Mo-N-Nb-Ni-O-P-Pb-S-Si-Sn-Ti-U-V-W-Zr) and pure FeO liquid, as well as for a greatly enlarged gaseous mixture phase and many stoichiometric solids and solid solution phases (within 30 elements: Ag-Al-Ar-B-C-Ca-Co-Cr-Cu-F-Fe-H-Mg-Mn-Mo-N-Na-Nb-Ni-O-P-Pb-S-Si-Sn-Ti-U-V-W-Zr). <u>Upgrade:</u> from SLAG1
ION2 TCS Ionic Solutions Database V2.0 (2002)	Based on ION1 (of 1992, with some modifications made in 1994 and 2001), many data for ionic liquid, metallic liquid, alloy solutions, and various oxide/silicate/sulfide/arsenide/carbide/nitride phases (stoichiometric solids and solid solutions) have been improved and added, and a greatly enlarged gas phase is included. Additionally, the critically-assessed data for Ag-Bi-Sr-Ca-Cu-O and La-Sr-O systems are combined, so it now covers 17 elements: Al-Ag-Bi-Ca-Cr-Cu-Fe-La-Mg-Ni-Si-Sr-O-C-N-S-As. <u>Upgrade:</u> from ION1
TCMP2 TCS Materials Processing Database V2.0 (2002)	Based on TCMP1 (<i>i.e.</i> , TCER of 2000), it is developed for applications to materials processing, to process metallurgy, and to chemical and waste-treatment processes (particularly materials recycling and remelting, as well as sintering, incineration and combustion). 5 more elements (Ag-Nb-U-V-W) are added, and thus totally 35 elements are covered now. Many data for liquid slag, metallic liquid, and various pure solid and solid solution phases have been improved and added. It also includes a greatly enlarged gaseous mixture phase. <u>Upgrade:</u> from TCMP1 (free for all TCMP users with TCC/TCW maintenance).
TCAQ2 TCS Aqueous Solution Database V2.0 (2002)	Based on TCAQ1 (of 1996, with minor modifications in 1999), it has been extended and modified by including more aqueous species involving Cu-Co-Ni-Zn-W. It now contains about 350 aqueous solution species, using the SIT model. <u>Upgrade:</u> from TCAQ1 (free for all TCAQ users with TCC/TCW maintenance).
MOB2 TCS Alloys Mobility Database V2.0 (1999)	Based on MOB1 (of 1995), it now contains assessed self- and impurity diffusion data for 75 elements, as well as assessed data for many binary, ternary and higher-order interaction alloy systems (in bcc, fcc, cementite, and Fe4N). <u>Upgrade:</u> from MOB1

Special discount offers are also available for the upgrades: from SSUB1 or SSUB2 to SSUB3, from SLAG1 to SLAG2, from ION1 to ION2, from TCMP1 to TCMP2, from TCAQ1 to TCAQ2, and from MOB1 to MOB2. For further information about upgrade of the databases, please contact info@thermocalc.se.

New Databases

Recently, several Thermo-Calc databases, as summarized in *Table 2*, have been made commercially available for new and add-on purchases.

Table 2. Some additional Thermo-Calc databases which are available now

Name & Version (Date)	Brief Descriptions
NSOL4 NPL Alloy Solutions Database V4.0 (2002)	Recently made available for use within TCC and TCW, it contains many critically-assessed thermodynamic data for non-ideal alloy solution phases, intermetallic phases and liquid mixture, within a 78-element framework.
NOX2 NPL Oxide Solutions Database V2.0 (2002)	Recently made available for use within TCC and TCW, it contains critically-assessed thermodynamic data for many oxide/silicate phases (both stoichiometric solids and solid solutions) and liquid oxide, in the Al-Ca-Mg-Fe-Si-O system.
NSLD2 NPL Solders Database V2.0 (2002)	Recently made available for use within TCC and TCW, it contains critically-assessed thermodynamic data for many Pb-free/-containing solder alloy solution phases in the Ag-Al-Au-Bi-Cu-Ge-In-Pb-Sb-Si-Sn-Zn system.
AQS2 TGG Aqueous Solution Database V2.0 (2002)	Recently made available for use within TCCP and TCW2.1, it connects the complete revised HKF model for aqueous solutions, that is applicable at temperatures up to 1000°C, pressures up to 5 kbar, and concentrations up to 6 molality (at room temperature and pressure) or higher (at high temperatures and pressures). It contains about 1500 free cations and anions, inorganic and organic complexes, within an 83-element framework. It can also be used in the POURBAIX module in TCCP software.
GCE2 TGG Geochemical & Environmental Database V2.0 (2002)	Recently made available for use within TCCP and TCW2.1, it contains critically-assessed thermodynamic data for about 600 minerals (silicates, oxides, hydroxides, halides, carbonates, sulfides, sulfates, nitrates, phosphates, and other rock-forming and environmentally-important minerals) within a 46-element framework. The compounds are treated as either stoichiometric or solution phases, over a wide range of temperatures, pressures and compositions.
NUMT2 UES Pure Radionuclides Database V2.0 (1999)	Recently made available for use within TCC and TCW, it contains 596 condensed and gas phase substances, including pure radionuclides in a 15-element system (Ba-Ce-Cs-I-La-Mo-Pd-Pr-Pu-Rh-Ru-Sr-Te-U-Zr), as well as other related pure substances (and gas mixture species) within a 44-element framework.
NUOX4 UES Nuclear Oxides Database V4.0 (1999)	Recently made available for use within TCC and TCW, it contains complete sets of assessed binary and ternary data in the UO_{2+x} - ZrO_2 - SiO_2 - CaO - Al_2O_3 - MgO - BaO - SrO - La_2O_3 - CeO_2 - Ce_2O_3 system for various nuclear applications.
SEM2 TC Semiconductors Database V2.0 (2002)	Recently made available for use within TCC and TCW, it contains all 15 possible binary subsystems and 18 ternary subsystems among the group III elements (Al, Ga and In) and the group V elements (P, As and Sb), as well as many gaseous species in the Al-As-Ga-In-P-Sb-Pb-Sn-C-H system.

Software License Upgrade

New versions of TCC, Thermo-Calc classic, and DICTRA are now released. For TCW we offer an option to our customers who already have a version of TCC to add a copy of TCW to their existing license. For further information about the license upgrade options please contact info@thermocalc.se

New License types

Two new license options are being introduced. The first option enables the customer to upgrade from an initial single license and have additional single licenses added. This type of license is offered at special rates for each additional license and is valid for the same site and with the same operating system as the initial license.

The second option is the possibility to get an annual license. This type of license runs for one year at a time and includes maintenance & support during the year.

Maintenance & Support

Maintenance & Support is provided to all new customers throughout one year (12 months). For continuous help after the initial year Maintenance & Support subscription is offered.

With effect from 2003 we have re-introduced one type of maintenance and support, providing the same level of assistance to all customer categories and license types. The Maintenance & Support subscription offers help to correct all known errors, automatic updates to new releases of the Programs and help and advice to use the Program in the most effective way. It also includes providing a new license file in case of switch of operating system, computer switch, computer crash or similar. Product documentation such as on-line manuals, technical documents, release notes and installation guides are also provided.

Training Courses

Our training courses guide the user how to apply the software capabilities in the most effective way. The courses provide hands-on exercises at the computers completed with short lectures. Dates and locations of forthcoming courses are shown below. For information and registration mail to ake@thermocalc.se.

Thermo-Calc Basic courses

The basic courses teach how to calculate phase equilibria, property diagrams and phase diagrams of alloys using TCC or TCW. Different types of phase diagrams such as isothermal and isoplethal sections are calculated. The systems treated are normally adapted to suit the participants interest.

- **TCC Basic** A basic course teaching the classical version of Thermo-Calc, TCC.
- **TCW Basic** A basic course teaching the windows version of Thermo-Calc, TCW.

The above courses are taught in parallel sessions.

Thermo-Calc Advanced course

The advanced course contains calculations including user-defined functions, liquidus surfaces. Calculations involving other types of systems such as oxides or gases are also performed. Thermodynamic databases and the use of programming interfaces are discussed. In this course we mainly use TCC.

DICTRA course

The course for new and experienced DICTRA users teaches how to perform different kinds of diffusion simulation problems using DICTRA. Multicomponent diffusion theory and the creation of mobility databases are also discussed in the course.

Training Courses in Stockholm, Sweden, Spring 2003

Courses:	Location:	Date:
TCW Basic	Stockholm, Sweden	7 May 2003
TCC Basic	Stockholm, Sweden	8 May 2003
TC Advanced	Stockholm, Sweden	9 May 2003
DICTRA	Stockholm, Sweden	12-14 May 2003

Short Courses at Penn State, USA

Penn State University is offering short courses designed to acquaint individuals in industry and academia with computational techniques now available in the areas of thermodynamics and kinetics.

Computational Thermodynamics and Thermo-Calc, May 5-6, 2003

In this course, fundamental thermodynamic principles will be reviewed in the framework of computational schemes. Hands-on experience will be provided, step by step, in interpreting practical cases in thermodynamic language and in implementing them in Thermo-Calc.

Diffusional Processing Simulation and DICTRA/Introduction to Phase-Field Simulation, May 7-8, 2003

The interplay of thermodynamics and element mobility/diffusivity will be presented for multicomponent systems in this course, using DICTRA, the general software package for simulation of DIffusion Controlled TRAnsformations in multicomponent system.

Thermodynamic and Kinetic Database Development with Thermo-Calc and DICTRA, May 9-10, 2003

This course is for people who would like to understand the thermodynamic database structure, and people who would like to modify or develop their own databases.

For more information about this program, please visit the Web site:
<http://www.outreach.psu.edu/C&I/Thermodynamics/>

User Group Meeting in Aachen, Germany

Our German agent ACCESS e.V. is organizing a Thermo-Calc/DICTRA User Group Meeting for old and new customers from German speaking countries in Aachen, Germany June 11-13. The first day will be reserved for a one day training course. The scope for the second and third day will be to exchange experiences and to present new features of Thermo-Calc and DICTRA. For detailed information about the program, deadlines for submitting a contribution, registration etc, please contact I.Steinbach@access.rwth-aachen.de.

Workshop on assessment of thermodynamic and kinetic data

To arrange a 3 days workshop or training session on techniques for assessment of thermodynamic and kinetic data using the PARROT module inside Thermo-Calc and DICTRA have been on our minds for some time. It is not possible to go into any details of this topic during our ordinary training courses, since most participants do not have this interest. However, we believe there are several users who would appreciate this kind of opportunity. Provided we can get a sufficient number of participants we plan to arrange such a workshop sometime during the autumn 2003. If you are interested in this, please let us know as soon as possible by sending an email to support@thermocalc.se.



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