



Thermo-Calc Software

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Software News

Since the formal release of the current versions of our software (TCCP, TCW2 and DICTRA22) and application programming interfaces (TQ4, TCAPI2 and TC Matlab-Toolbox 2) early this year, many clients have started using these packages successfully in their R&D projects and teaching activities. Some patches of the software and interfaces have been provided through our web site. Our further developments for the next major releases (TCCQ, TCW3 and DICTRA23; TQ5, TCAPI3 and TC Matlab-Toolbox 3) have been progressing smoothly as planned.

Download the Latest Patches

New patches (the latest updated sub-versions of a software or interface) have been recently made available for downloading from our web site. These patches include further improvements and bug fixes that have been made after the release of the current version. With a valid license for the current version of a specific software/interface, you can download and install such a patch. We encourage all users to regularly check for such new patches at www.thermocalc.com/download/updates.html.

Successful Applications of Programming Interfaces

The TQ, TCAPI and TC Matlab-Toolbox have been efficiently applied by many of our clients, for complex materials property calculations and materials process simulations. We highly appreciate such partners to share their successful stories with us and our other customers.

In the Thermo-Calc Newsletter No 26, the **MICRESS™ software**, developed by ACCESS e.V., Aachen, Germany, was described. It couples the Phase Field approach and TQ4 interface, and is very powerful to simulate microstructure evolutions of multicomponent alloys, especially in considering phase transformation kinetics. For more details on the MICRESS software and applications, please visit www.access.rwth-aachen.de.

Two other distinguished examples are briefly introduced below:

PrecipiCalc™ Software

It is a sophisticated computer program developed by QuesTek Innovations LLC, USA, for calculating the 3D multiparticle diffusive precipitation kinetics of multiple phases. It adopts multicomponent thermodynamics and diffusion based on the CALPHAD approach, through the incorporation of TCAPI. This allows realistic and mechanistic modeling of nucleation, growth, and coarsening without resorting to *ad hoc* treatments. The incorporation of TCAPI allows access to the thermodynamic and kinetic quantities of complex alloys boosting the numerical efficiency and accuracy of the software.

The primary input of *PrecipiCalc* software includes:

- Physical quantities such as material compositions, bulk thermodynamics and mobility (TDB files), interfacial properties (e.g., surface energy), lattice properties (e.g., molar volume);
- Thermal cycle, or temperature profile, which defines the thermal history of the material being processed. The thermal cycle can be constant (isothermal), linear cooling (quench), or as complicated as nonlinear and non-monotonic heat treatment (such as multi-step tempering).

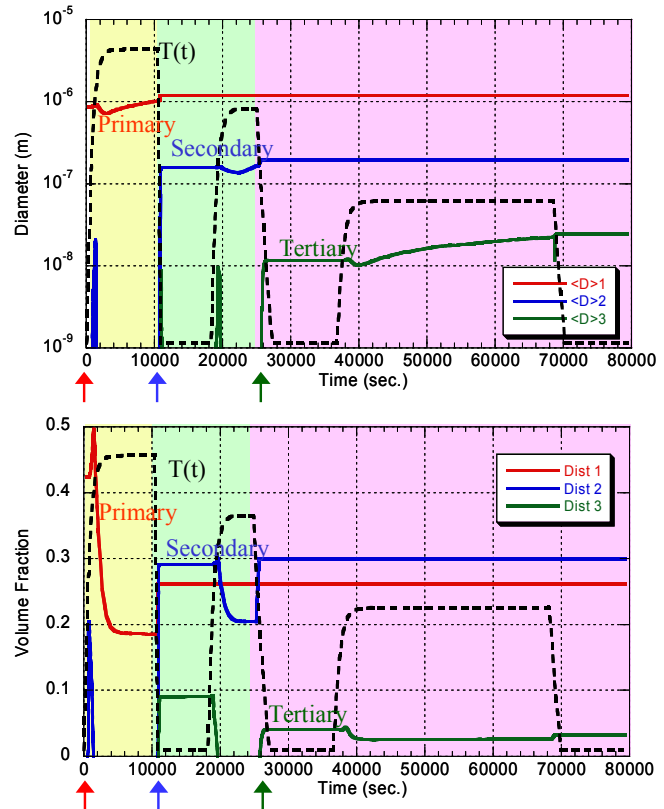
The output of *PrecipiCalc* software includes the time evolution of

- Precipitate microstructure — precipitate size distribution, number density and fraction;
- Compositions of matrix and precipitate;
- Driving forces, nucleation rates, and critical radii.

PrecipiCalc has been successfully applied to the design and process optimization of a wide range of metallic systems, including γ' and carbide/boride precipitation in Ni-based superalloys, carbide/nitride/intermetallic precipitation during welding and heat treating in steels, FCC devitrification in amorphous Al-based metals, and Heusler phase in NiTi-based shape memory alloys.

The two plots shown here illustrate an example of *PrecipiCalc* γ' precipitation calculations for an aeroturbine disk Ni-based superalloy, IN100, under a complex commercial heat treatment. Three distinct γ' particle size distributions within a range of size scales (10nm to 1 μ m) are observed experimentally and validated in this calculation. Integrating the *PrecipiCalc* calculations with a FEM heat transfer simulation and a mechanistic strength model allows the spatial microstructure/property variation in the disk to be determined. This evaluates uncertainty and variation of the alloy properties within the disk, a valuable tool in accelerating the qualification of the alloy in this critical application. Such complex calculations would be significantly more difficult without access to underlying thermochemical and kinetic quantities that the TCAPI provides.

For more information about the *PrecipiCalc* software and applications, please contact Dr. Heng-Jeng Jou, hjjou@questek.com.

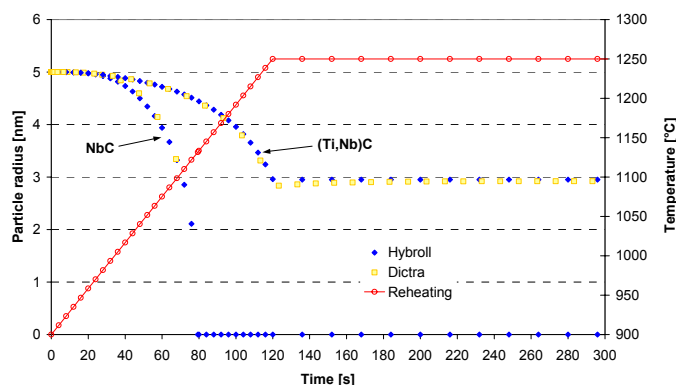


Applications of TC Matlab-Toolbox in Process Simulation at SSAB Tunplåt

At SSAB Tunplåt in Borlänge, Sweden, a system for prediction of mechanical properties in hot rolled products, Hybroll, is under development. The work started as a multipartner ESCS project ("The prediction of the mechanical properties of hot rolled strip products using hybrid methods", ESCS Project #7210-PR-164). The system is designed for materials that cover C-Mn steels, HSLA steels with Nb, Ti and V additions and high carbon steels.

The microstructural model calculates a microstructure after hot rolling. Inputs to the model are time, temperature and strain sequence during hot rolling. This calculated microstructure is then used as input to the flow stress model. The flow stress model calculates a stress-strain curve from which $R_{p0.2}$, R_m and A_g can be evaluated directly. The different sub-models describing the microstructural evolution during hot rolling are particle dissolution and precipitation, grain growth, recrystallisation, the evolution of dislocations and vacancies, the transformation from austenite to ferrite and eutectoid and the description of flow stress. The models must be fast enough to be able to run on process computers, but still give a reasonably general description of the microstructure evolution. Both experimental data taken from literature and laboratory experiments are used for model tuning. During the model development, the Matlab™ software has been used.

To predict the driving force and supersaturation in the matrix, as well as the paraequilibrium that occurs during the decomposition of austenite, thermodynamic data is needed. The



thermodynamic data is taken directly from the Thermo-Calc software using the TC Matlab-Toolbox. A specially developed database for HSLA steels is used for the calculations.

This figure shows a particle dissolution during a heating sequence. The HYBROLL model is compared to the DICTRA software for NbC and (Ti,Nb)C particles, and the deviation between these two is negligible.

Database News

Several databases are now available in updated versions, and are also offered at certain discount rates for database upgrades from their older versions (e.g., from TCFE2 to TCFE3, from SSUB2 to SSUB3, from SLAG1 to SLAG2, from ION1 to ION2, from TCAQ1 to TCAQ2, and MOB1 to MOB2, etc.). For further information about the upgrade options, please refer to the last edition of Thermo-Calc Software Newsletter (No 27, published in April, 2003) or contact info@thermocalc.se.

Some new Thermo-Calc databases are introduced to our customers, described below. For more details of such databases and their applications, please refer to the Database Description Forms documented in the Thermo-Calc and DICTRA Users Guides and our web site, or please contact info@thermocalc.se.

- Thermo-Calc Software has further developed and completely revised the TCMaterials Processing Database (**TCMP2**), for applications in materials processing, process metallurgy, and chemical and waste-treatment processes (particularly materials recycling and remelting, as well as sintering, incineration and combustion). It covers 35 elements (Ag-Al-Ar-B-Bi-C-Ca-Cd-Cl-Co-Cr-Cu-F-Fe-H-K-Mg-Mn-Mo-N-Na-Nb-Ni-O-P-Pb-S-Sb-Si-Sn-Ti-U-V-W-Zn). Many types of multicomponent compound and solution phases are available, such as: melt (metallic/non-metallic liquid mixture), slag (oxide/silicate/sulfide/phosphate/fluoride... liquid mixture), gas (gaseous mixture), metallic/non-metallic solid solutions, and many stoichiometric solids (e.g., metals, oxides, hydroxides, silicates, sulfides, sulfates, nitrates, nitrites, phosphates, phosphites, carbonates, borates, halides, and other inter-metallic/non-metallic compounds).
- SGTE (Scientific Group Thermodata Europe) has recently updated the SSOL Alloy Solutions Database (to version 4.0, **SSOL4**). Many new and revised phases, phase descriptions and related parameters have been incorporated into this updated version, and thus it is more general and useful for applications in various types of alloy material systems and processes. Thermo-Calc Software offers special discounts to our clients to upgrade from an older version of the SSOL database (SSOL1 or SSOL2).
- SGTE has also adopted the SNOB Noble Metals Database (version 1.0, **SNOB1**), which has been developed by Spencer Group, USA, in cooperation with GTT Technologies, Germany. It is especially designed for applications of R&D of noble metal alloys, for instance, jewellery and decoration, electronic components, micro-electronic contact materials, solders and brazes, dental alloys, fission products, catalysts, new minority alloy components (e.g., in turbine alloys), scientific equipment (e.g., thermocouples, crucibles, calorimeters). It contains evaluated thermodynamic data for noble metal alloys of Ag-Au-Ir-Os-Pd-Pt-Rh-Ru, both alloyed amongst themselves and in alloys with other elements (Al-As-Bi-C-Co-Cr-Cu-Fe-Ge-In-Mg-Ni-Pb-Sb-Si-Sn-Ta-Te-Ti-Tl-Zn-Zr).

Additionally, all ten public Thermo-Calc databases have been recently renamed and updated (*i.e.*, **PURE4**, **PSUB**, **PBIN**, **PTERN**, **PION**, **PKP**, **PCHAT**, **PG35**, **PGEO** and **PAQ2**). Any such database with binary, ternary or high-order interaction parameters for alloy solutions can be directly used now, both in the BIN and TERN modules of the TCC software and in the Binary Phase Diagram module of the TCW software. They will be included without any change in new distributions of the TCCP/TCW2 software and in the updated TCCP-Demo/TCW2-Demo package that will be available soon for downloading from our web site, and of course in next TCC/TCW software release.

Company News

New Web Site

Thermo-Calc Software has recently launched a new edition of its web site. The front page has been rearranged and redesigned with new and easy-to-use headings and sub-headings, which will increase the user-friendliness of the web site and enable us to provide our visitors with an improved guide to various products and services. Several updated and new features, as well as the latest patches, site map, search facility, licensing and computer requirements, ordering option forms, etc., have also been added. You are most welcome to regularly visit www.thermocalc.com.

New Distributors

China

It is our pleasure to announce that we have made an agent agreement with Professors Yong Du, Zengpeng Jin and Huashan Liu at the Central South University in Changsha to act as our agent in China. For further information, please see contact details on our web site.

Thermo-Calc Software, Inc., in North America

ESI Software (formerly UES Software) will, as of November 30th 2003, no longer act as our distributor in North America. This is an important and demanding market for us, and we have decided to establish a fully-owned subsidiary of ours, **Thermo-Calc Software, Inc.**, in order to ensure that all our US customers receive proper guidance and support. The subsidiary will be fully backed-up by the main office in Sweden, which should guarantee quality service at all times. Our subsidiary will be operational as of February 1st 2004 and located at 4160 Washington Road, McMurray, PA 15317, USA. In the interim all customers will be supported directly from the main office in Sweden. For more information, please contact Dr. Anders Engström (anders@thermocalc.se).

New Staff

Dr. Qing Chen recently joined our Product Development Section. He has a Ph.D. degree in materials science and engineering. After graduating from Central South University in China in 1995, he has worked as research scientist at KTH (Stockholm), and Ohio State University (Columbus). He is an expert on phase diagrams, phase transformations and microstructure modelling, and his main scientific interests have included developing thermodynamic databases for synthesizing functional oxide crystals, establishing method to model defects and electronic properties in compound semiconductors, linking first principles calculation with CALPHAD and modelling thermophysical properties with physical parameters, and phase transformations and microstructure simulations on real length and time scales using Phase Field Method coupled with Thermo-Calc and DICTRA. He is one of the principal developers of the SCHEIL module and TQ interface.



Ms. Hillevi Tobrand joined our Finance Section several months ago. She is specialized in finance handlings and customer relations.



Upcoming Events

MS&T Conference and Exhibition

Please meet us at the MS&T Conference and Exhibition in Chicago, IL, USA, for a discussion or any issue concerning our products and services. You will find us in the Exhibition Booth 301, during Nov. 9-11, 2003.

Assessment Courses and Graduate Courses in Computational Thermodynamics

An assessment course (using PARROT for optimization of model parameters to fit experimental and theoretical data) will be given during the week 48, 2003, under the supervision of Prof. Bo Sundman at MSE, KTH, Stockholm. E-mail to ake@thermocalc.se if interested. There are also plans for arranging graduate courses, teaching how to use Thermo-Calc, to understand thermodynamic models for different types of phases, and to perform assessments; please visit www.web.mse.kth.se/bosse/ccepd.html to know more.

Thermo-Calc Day and DICTRA Training Course in Tokyo

CRC Solution Inc. (our agent in Japan) is going to hold the third **Thermo-Calc Day** (December 2nd, 2003) and DICTRA training course (December 3rd-5th, 2003) in Tokyo. Two representatives of Thermo-Calc Software will join the event. If interested, please contact Dr. Satoshi Minamoto (s-minamoto@crc.co.jp).

TCC, TCW and DICTRA Training Course in Stockholm

The forthcoming combined TCC/TCW/DICTRA course will be given in Stockholm, during April 21st-28th, 2004, as announced on our web site. For information and registration, please mail to Dr. Åke Jansson (ake@thermocalc.se).



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