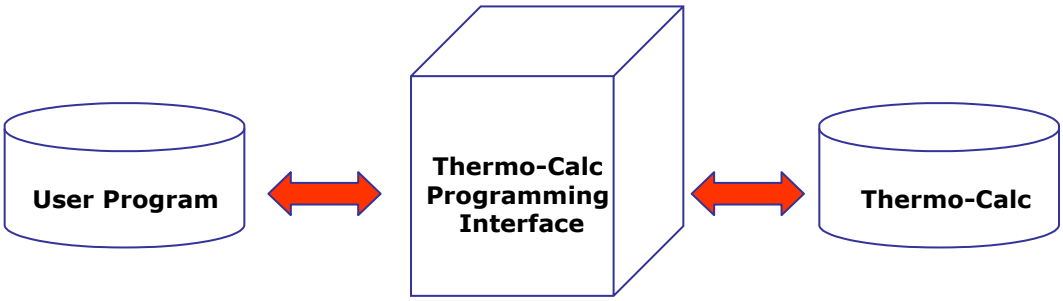
Thermo-Calc Programming Interfaces: TC-PI



Thermo-Calc Programming Interfaces (TC-PI) are available for advanced users who want to further extensively use the power and flexibility of the Thermo-Calc software in their own application programs or within a third-party software package. Three different programming interfaces are available now: TQ, TCAPI and TC-MATLAB® Toolbox. Without having to implement various sophisticated models or mathematical routines, or have extensive knowledge of Thermo-Calc, and possibly through coupling with such phase-field methods, fluid-dynamic approaches and other modeling technologies, one can use these programming interfaces for retrieving thermodynamic data (as well as diffusion coefficients) and for calculating phase equilibria, directly within user's own application programs or third-party software packages, not only for various user-specified thermodynamic calculations but also for advanced simulations of materials processing, microstructural evolution, physical properties, mechanical properties, and so forth. Among the most distinguished and successful application examples of these programming interfaces are the recently-developed MICRESS™, PrecipiCalc™ and TC-PRISMA™ software packages.

Through the programming interfaces, most of the quantities that are available from the Thermo-Calc software can be obtained, *e.g.* temperature, pressure, volume, chemical potential, phase amount, phase composition, partition coefficients, liquidus or solidus points, invariant temperature, heat of reaction, adiabatic combustion temperature, and even diffusion coefficients when used in conjunction with a suitable mobility database such as MOB2, MOBFE2, MOBNI2 or MOBAl2. Furthermore, calculations can not only be applied to equilibrium calculations but can also be used to predict metastable or non-equilibrium or para-equilibrium states by changing the status of the phases under consideration.

Examples of quantities and properties that can be calculated using the Thermo-Calc Programming Interfaces are:

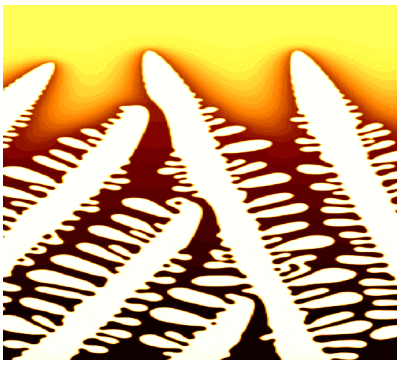
- Amount and composition of phases
- Phase transformation temperatures, such as liquidus and solidus temperatures
- Thermochemical properties, *e.g.* C_P , ΔH
- Driving forces
- Diffusion coefficients
- Derivatives of state functions, *e.g.* $\frac{\partial G_m^\theta}{\partial x_i}$, $\frac{\partial^2 G_m^\theta}{\partial x_i \partial x_j}$
- Partition coefficients
- Invariant temperatures, liquidus-/solidus- temperatures and composition-dependence
- To-temperature, A1/A3/A4-temperatures, adiabatic temperature, chill factors, composition derivatives of temperature, *etc.*
- Thermodynamic limits for partitionless transformations and for transformations under para-equilibrium and quasi-paraconditions
- *… and many more …*

"TC-PI provides a simple and efficient way to insert thermodynamic and kinetic data into modeling of materials processing, microstructural evolution, and physical-mechanical properties."

TQ Interface (TQ)

The TQ is written in FORTRAN for application programming under almost all available CPU environments, *e.g.* PC-Windows, PC-Linux, UNIX platforms (Sun, Solaris and SGI IRIX). It is designed for time-critical, computationally-intensive application software that are most likely but not necessarily written in FORTRAN.

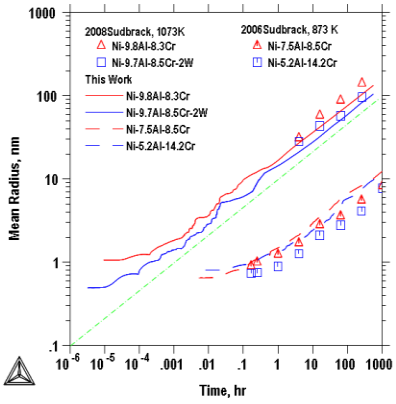
The TQ has been successfully implemented also in the MICRESS™ software package (developed by ACCESS e.V., in Aachen, Germany), for simulation of microstructural evolution in multicomponent alloys using the phase-field approach. The TQ provides MICRESS® with a reliable thermodynamic and kinetic basis when simulating microstructures in multicomponent alloys in varied materials processes.

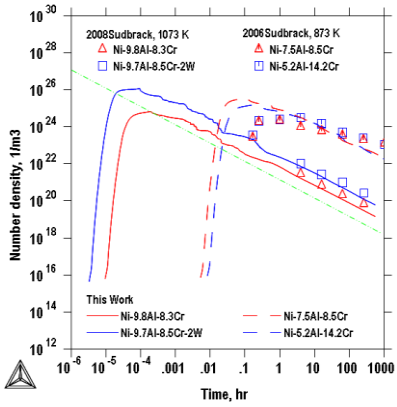


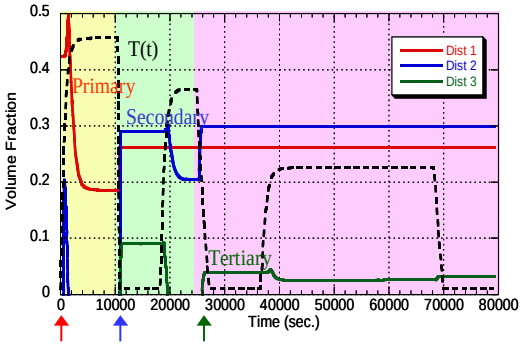
Thermo-Calc Application Programming Interface (TCAPI)

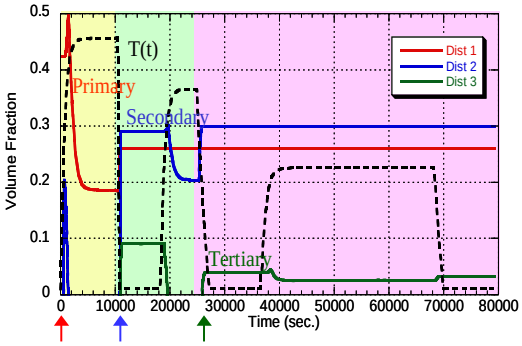
The TCAPI is written in C for programming under PC-Linux and PC-Windows environments. Thermo-Calc for Windows (TCW) and the TC-MATLAB® Toolbox are actually based on this programming interface.

Since the TCAPI is written in C, linkage to and communication with programming languages other than FORTRAN is more convenient compared to the TQ. Also, the TCAPI includes more of the functionality available in the Thermo-Calc software. It offers access to most of the commands in the TDB, POLY3 and POST-processor modules and to some important commands in the GES5 module. The TCAPI is most suitable for developing Windows-based applications involving advanced thermodynamic and/or kinetic calculations. For example, the TCAPI has been incorporated in the software package PrecipiCalc™, for precipitation calculation in Materials/Process Design and Optimization (developed by QuesTek Innovations LLC in USA). The PrecipiCalc™ is a sophisticated computer program for calculation of precipitation kinetics in materials with multiple particles and phases. The incorporation of the TCAPI allows access to thermodynamic and kinetic quantities of complex alloys and hence use of realistic and mechanistic models without resorting to ad hoc treatment. The PrecipiCalc has just recently become an entirely-merged part of our newest software package TC-PRISMA™, which has also used the TCAPI for the interconnections with the Thermo-Calc and DICTRA software/databases.







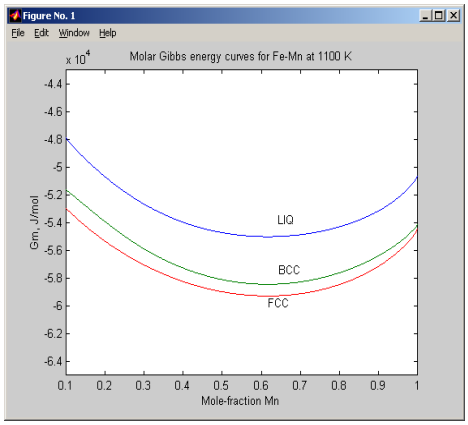


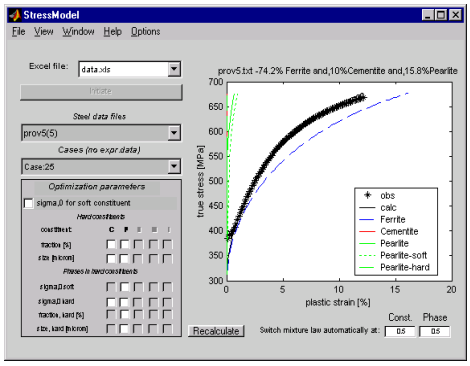
TC-MATLAB® Toolbox

The third addition of the Thermo-Calc Programming Interfaces group (TC-PI) is the TC-MATLAB® Toolbox, which provides a programming interface to the commonly-used MATLAB® software for scientific and engineering computing. At present, the TC-MATLAB® Toolbox is only available for the PC-Windows environment.

MATLAB® is a very flexible software for technical computing and visualization of data. The software comes with more than 600 mathematical, statistical and engineering functions and great graphical capabilities. It can be considered as a matrix-oriented programming language and contains compilers, links and libraries for different scientific applications. This flexibility is now enhanced even more with the possibility to retrieve thermodynamic and kinetic quantities through the TC-MATLAB® Toolbox. This programming interface is ideal for fast realization of ideas and visualization of results during research and development activities.

In the current version of the TC-MATLAB® Toolbox, more than 50 commands are available for application programmers, including a set of commands also for communicating with the DICTRA software. The TC-MATLAB® Toolbox has been used in a process simulation model developed at SSAB Tunnplåt in Borlänge, Sweden. The model, containing a whole range of sub-models, is used for prediction of mechanical properties in hot rolled products.





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