



Thermo-Calc Classic

Thermodynamics at your fingertips

1 Introduction

Thermo-Calc Classic (TCC) is the classical version of the general and flexible software Thermo-Calc, which has gained world wide reputation as the best software for calculations of multicomponent thermodynamics and phase diagrams. Today there are more than 1000 installations of TCC all over the world, in both academic institutions and industry.

TCC is a highly versatile software, which has multiple applicability in the field of materials science and engineering. If metal production is used as an example, then TCC can perform calculations that are of interest for:

- Ore sintering
- Pyrometallurgic reactors
- Casting and microsegregation
- Alloy design, systematic development of new materials
- Electrochemical processes, Pourbaix diagrams
- Gas-Metal reactions
- Gas compositions, carbon potentials, oxygen potentials
- Thermophysical properties, C_p , ΔH , volume, etc.

Thermo-Calc Classic is ideal software for these purposes as it can handle many components, *i.e.* "real" materials and all their thermodynamic properties.

2 The Thermo-Calc Classic software

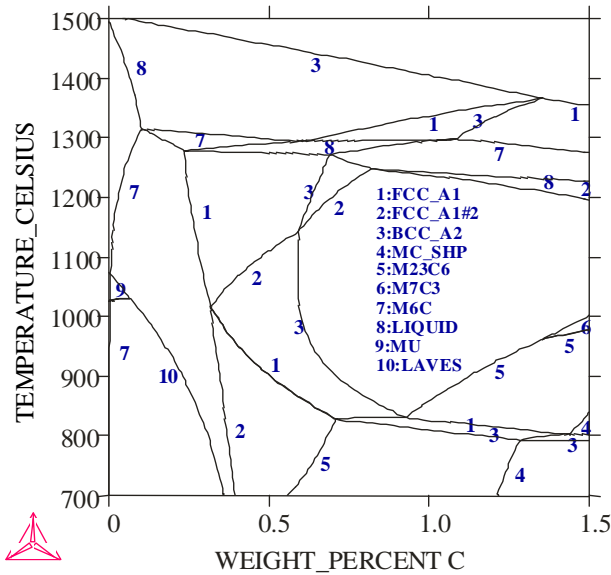
After more than 30 years of developing and refining Thermo-Calc Classic, we are proud to offer what we believe is the world's best software for thermodynamic calculations. Incorporated in Thermo-Calc Classic are numerous models for thermodynamic properties of elements, compounds, solid solution phases, liquids, aqueous solutions, gaseous mixtures, polymers and more. The combining of this with a powerful calculation engine and a flexible post-processor, Thermo-Calc Classic is capable of performing many calculations of interest in materials science and engineering.

Applications

- Phase diagrams (binary, ternary, isothermal, isoplethal, *etc.*) (*up to 5 independent variables*)
- Thermodynamic properties of pure substances, compounds and solution phases
- Thermodynamic properties of chemical reactions
- Property diagrams (fraction of phases, Gibbs energy, enthalpy, C_p , volume, *etc.*) (*up to 40 components*)
- Pourbaix diagrams and many other diagrams for aqueous-involving interaction systems
- Partial gaseous pressures, chemical potentials of volatile species (*up to 1000 species*)
- Scheil-Gulliver solidification simulations and its extension by considering interstitial back diffusion in solid phases
- Liquidus surfaces for multicomponent alloys
- Thermodynamic factors, driving forces
- Heterogeneous equilibria (*up to 40 components*)
- Metastable equilibria, para-equilibria
- Transport properties of aqueous solutions
- Special quantities: *e.g.*, T_0 , A_3 -temperature, adiabatic T, chill factors, $\partial T/\partial X$, *etc.*
- Oxide-layer formation on steel surfaces, steel/alloy refining, so-called PRE numbers
- Evolution of hydrothermal, metamorphic, volcanic, sedimentary, weathering processes
- Speciation in corrosion, recycling, remelting, sintering, incineration, combustion
- CVD diagrams, thin-film formation
- CVM calculations, chemical ordering-disordering
- Thermodynamics of steady-state reactors
- Establishment and modification of datasets or databases
- Simulation of Carnot cycles
- "*Anything you can think of which represents an equilibrium ...*"

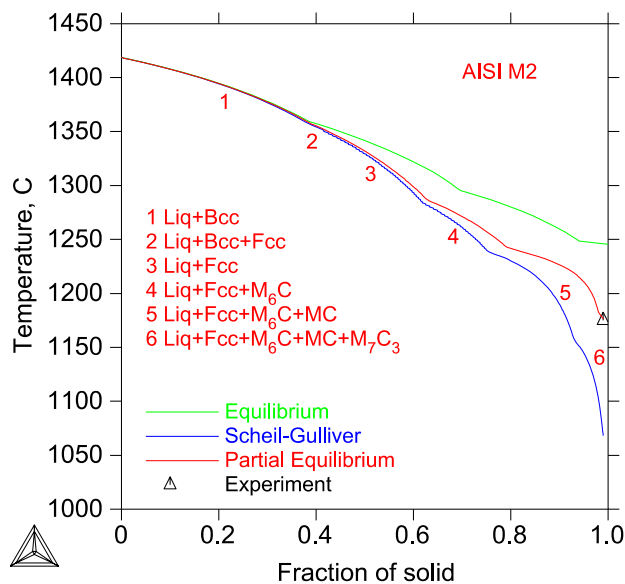


Since Thermo-Calc Classic can handle multicomponent systems, it is easy to investigate how a change in the content of an alloying element affects the stability of different phases, by calculating a property diagram or a phase diagram (shown below is a phase diagram for a tool steel):



Phase diagram for a tool steel. The lines represent where a phase appears or disappears, numbers show on which side of the line that phase is present. The composition is Fe-4Cr-5Mo-8W-2V-0.3Mn-0.3Si-C (wt-%).

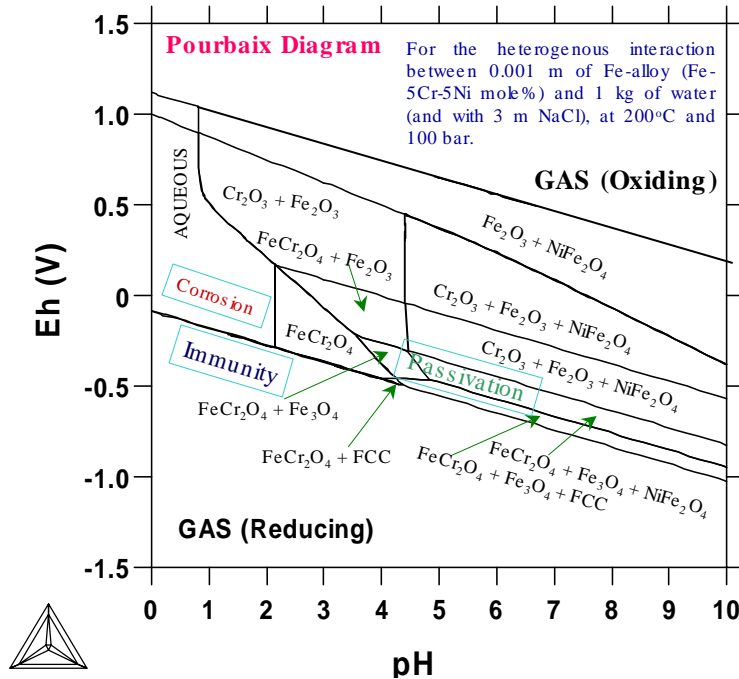
Thermo-Calc Classic is also capable of performing process simulations, e.g. solidification path and microsegregation in multicomponent alloys using the Scheil-Gulliver model (which has been further improved by considering interstitial back diffusion in solid phases and allowing BCC→FCC phase transformation during solidification), as illustrated below:



Results (on a plot of temperature vs. mole fraction of solid phases) from the Scheil-Gulliver simulation for an Fe-3.9Cr-0.36Ni-0.3Si-0.32Mn-4.9Mo-0.3Co-0.1Cu6.1W-1.9V-0.88C (wt%) alloy. The plotted diagram shows solidification path, using three different approaches: Equilibrium stands for level-rule (full equilibrium) calculation; Scheil-Gulliver for traditional Scheil-Gulliver simulation; and Partial Equilibrium for modified Scheil-Gulliver simulation (where back diffusion of the C component and BCC→FCC transformation are considered). The experimental data on measured freezing range on the specified steel is compared well with the simulated result using the Partial Equilibrium approach (which is particularly useful for various steels).



With Thermo-Calc Classic, it is also possible to make calculations including aqueous solutions such as the Pourbaix diagram below. Such calculations are applicable in corrosion, hydrometallurgy, geochemistry and environmental issues among others. The interaction between a multicomponent alloy and an aqueous solution can be calculated this way.



Pourbaix diagram for 0.001 m of Fe-alloy (Fe-5Cr-5Ni mol%) actively reacted with 1 kg of water (and with 3m NaCl) at 200°C and 100 bar. The diagram shows various stable phase regions for FCC-alloy phase, aqueous solution, gaseous mixture and varied types of oxides.

2.1 Databases

The Thermo-Calc Classic calculations are based on thermodynamic databases created by critical assessments of experimental data. Today there are accurate thermodynamic data available for many different types of materials such as:

- Steels (stainless steels, HSLA steels, high-speed steels, cast irons, among many other types)
- Ni-/NiFe-based superalloys
- Ti-/TiAl-based alloys
- Al-based alloys
- Mg-based alloys
- Zr-based alloys
- Solder alloys (Pb-bearing/-free)
- Semiconductor alloys
- Nuclear materials
- Hard materials, ceramics
- Slags
- Molten salts
- Minerals
- Aqueous solutions
- Gaseous mixtures

For detailed and actual information regarding available databases, see our homepage www.thermocalc.com.

2.2 Output Facilities

Thermo-Calc Classic has a post processor for producing output from the simulations. Graphs are easily plotted with different axis variables. It is easy to incorporate a calculated diagram in a report using one of the many graphical formats that are supported e.g. EMF, PNG, BMP, PDF, JPEG, TIFF, PostScript, HPGL, HP-Laserjet, Regis, etc. The coordinates of the plot can also be tabulated in e.g. MS Excel file to be processed by other software.



2.3 Use Thermo-Calc in your own software

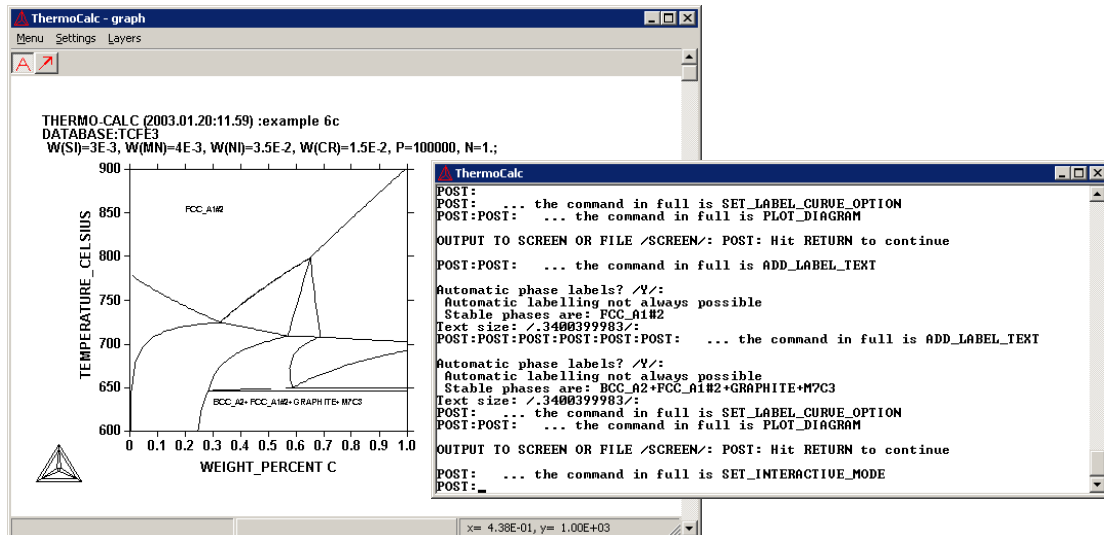
It is also possible to use Thermo-Calc in your own software through the application programming interfaces. This technique utilizes the Thermo-Calc engine to calculate various thermodynamic properties, while you can focus on other problems. More information on the programming interfaces is available on our homepage www.thermocalc.se.

2.4 User Interface

The Thermo-Calc Classic software is divided into several different modules for performing different tasks e.g. retrieving data, performing a calculation or plotting the results. The user interface consists of a command line interface where commands are typed. All commands can be abbreviated for convenience. There are also special modules for certain types of calculation such as Scheil-Gulliver simulations of solidification and calculation of Pourbaix diagrams for aqueous-bearing interaction systems.

After gaining some experience with the software, it is extremely easy to construct interactive **MACRO** files, which performs a TCC calculation. Using **MACRO** files makes it possible to save complicated command sequences and repeat them many times for different cases at different times.

There are complete help facilities for the users. A list of available commands can be retrieved by simply typing a question mark ? at the command prompt and there are also descriptions of all commands available.



The user interface of TCC

2.5 Availability of Thermo-Calc Classic

The TCC software is available for PC computers with the O/S Microsoft Vista Business/XP or Linux