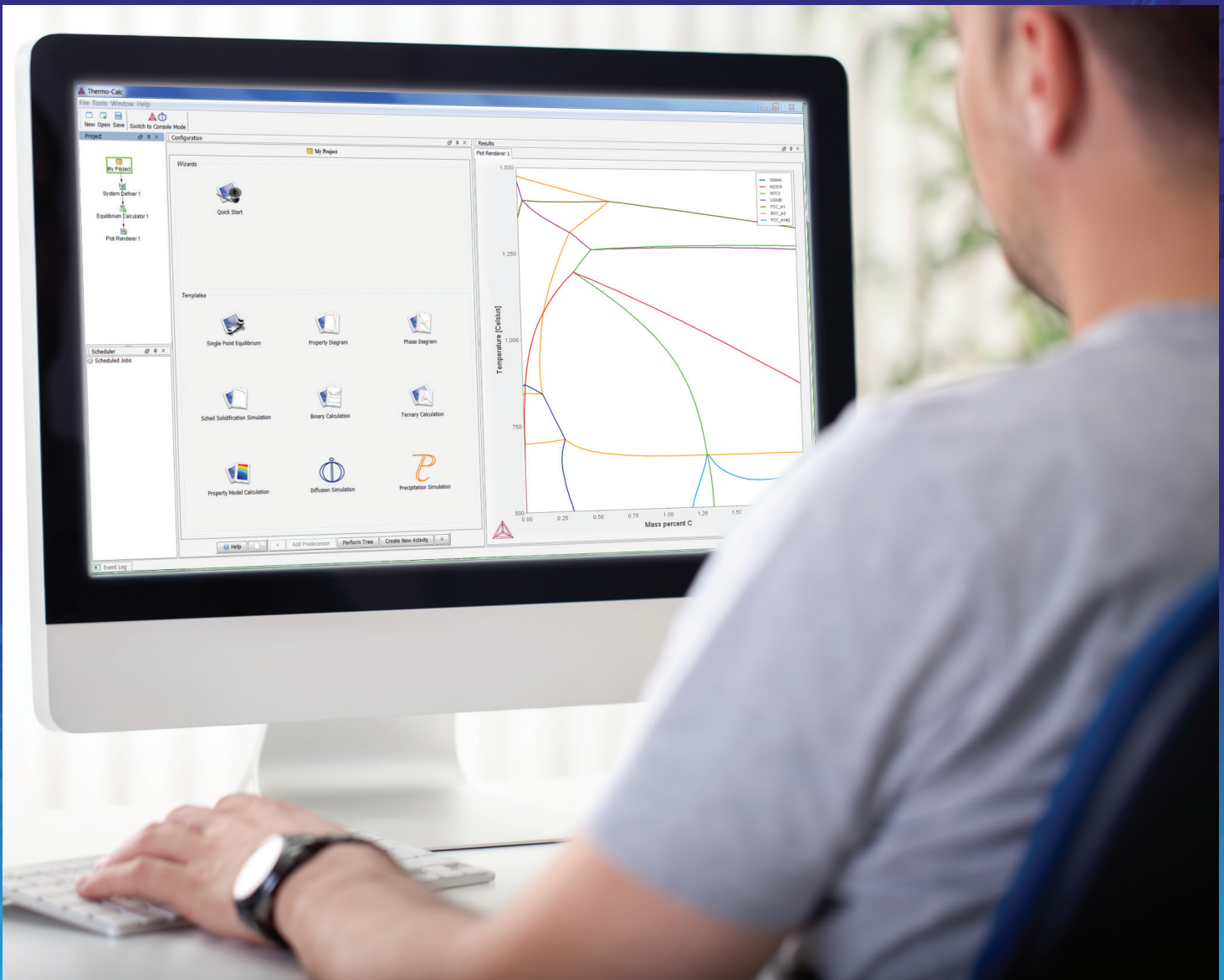


Thermo-Calc Software

Powerful Software for Computational Materials Engineering

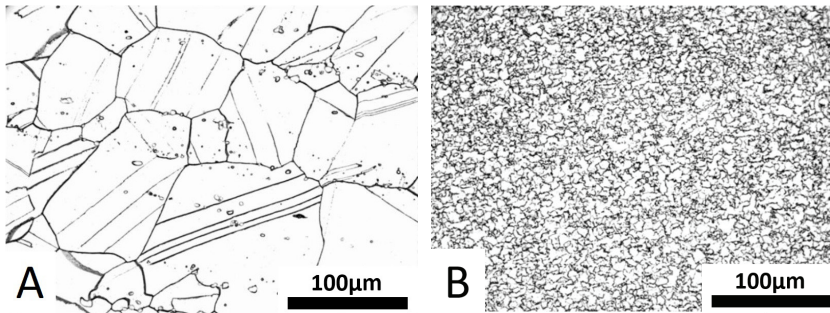
Applications to Heat Treatment



Get the Materials Data You Need with Thermo-Calc

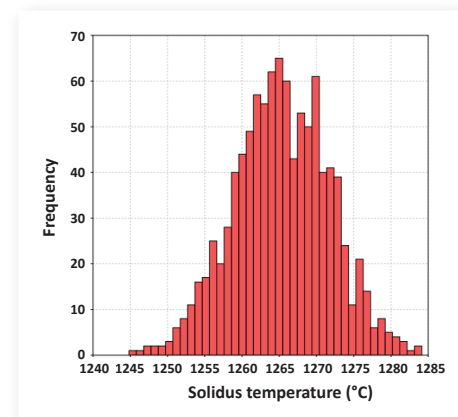
Materials are complex systems where microstructure and properties can vary depending on:

Processing Conditions



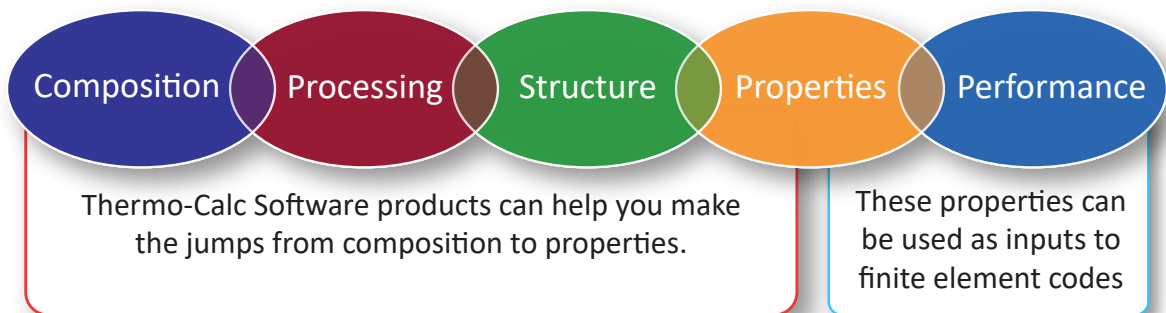
Grain size comparison of Hastelloy® X
(A) Wrought
(B) Friction Stir Processed

Composition



Variation in solidus temperature over 1000 compositions within alloy 718 specification

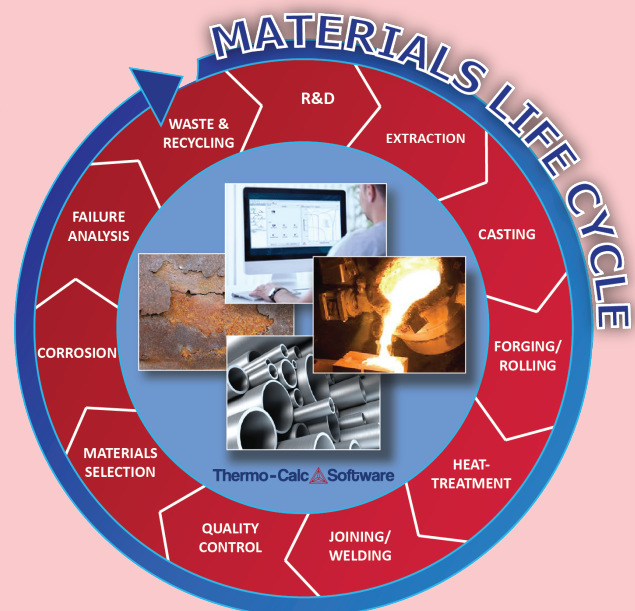
Integrated Computational Materials Engineering (ICME) is transforming the way scientists and engineers think about materials by linking composition and processing conditions to material properties, a critical component of understanding part performance and material design.



ICME requires materials data at all stages of the materials life cycle:
What do you do when that data doesn't exist?

With Thermo-Calc You Can:

- ✓ **Calculate** thermodynamic and phase-based properties as a function of composition, temperature and time
- ✓ **Fill in** data gaps without resorting to costly, time-consuming experiments
- ✓ **Predict** how actual vs nominal chemistries will affect processing windows
- ✓ **Base decisions** on scientifically supported models
- ✓ **Troubleshoot** issues during materials processing
- ✓ **Accelerate** materials development while reducing risk



Solidification and Homogenization

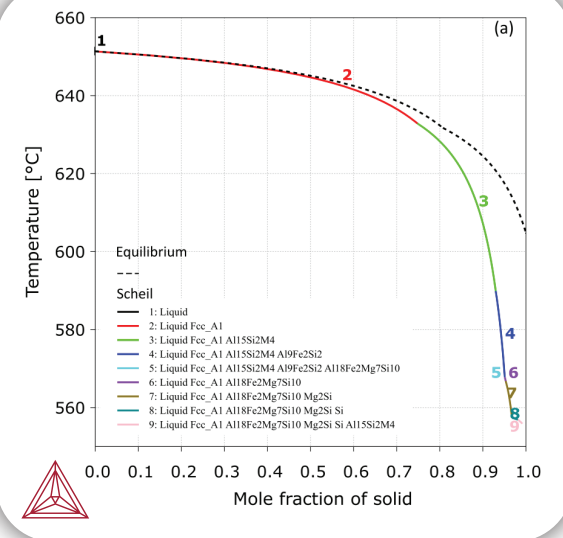
Calculate solidification segregation

Thermo-Calc can be used to calculate the solidification behavior of alloys under equilibrium and non-equilibrium conditions.

With Thermo-Calc you can calculate:

- The solidification range of an alloy
- Depression of the solidus temperature due to microsegregation
- Composition of the last liquid to solidify in the interdendritic region
- Phases formed on final solidification in segregation pockets
- The composition gradient across a hypothetical dendrite

The calculation on the right shows both the equilibrium and non-equilibrium solidification path of Aluminum AA6005.

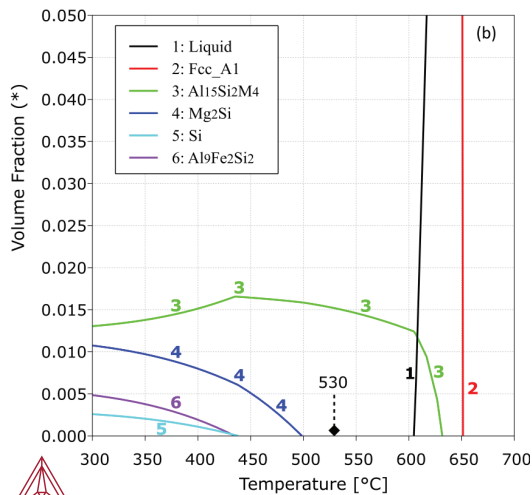


Determine homogenization temperature

As shown above, undesirable precipitates may form during solidification. The stability of these phases as a function of temperature and their solvus temperatures can be calculated.

The equilibrium calculation on the left illustrates this for the same AA6005 alloy.

Heat treatments can then be determined at temperatures above the solvus temperature to dissolve these precipitates.

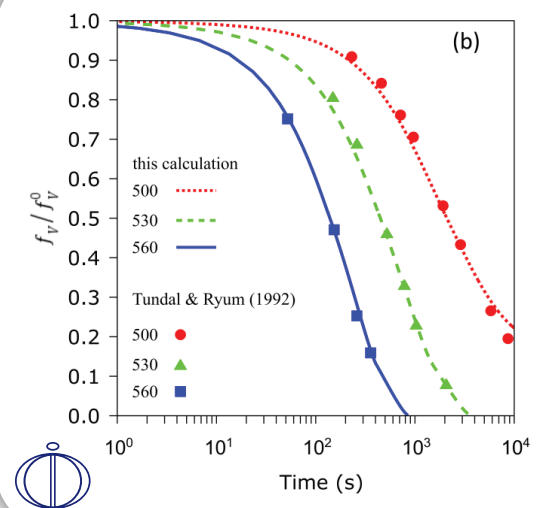


Predict time needed to homogenize

The diffusion module in Thermo-Calc allows kinetic calculations to be performed as a function of temperature, time, and distance.

This can be used to predict the time required to homogenize a segregated composition profile and dissolve undesirable precipitates.

The figure to the right shows how quickly the precipitates dissolve at different temperatures in the solidified AA6005 alloy.



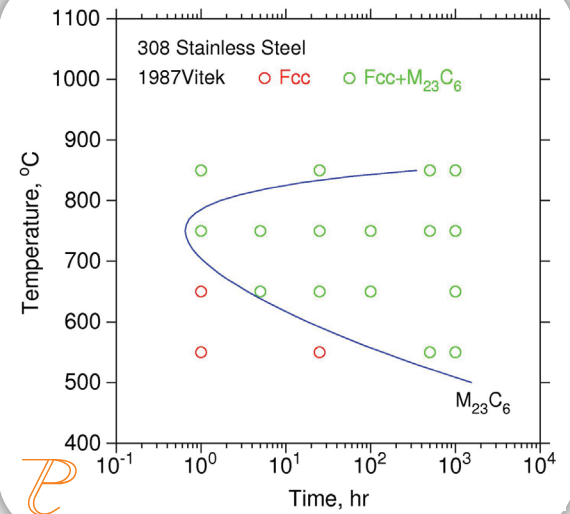
Aging and Precipitation

Generate TTT diagrams for specific chemistries

The Precipitation Module can predict the concurrent nucleation, growth/dissolution and coarsening of precipitate phases as a function of time and temperature under isothermal and on isothermal conditions.

One use of this module is to predict TTT and CCT diagrams for precipitate phases as a function of chemistry.

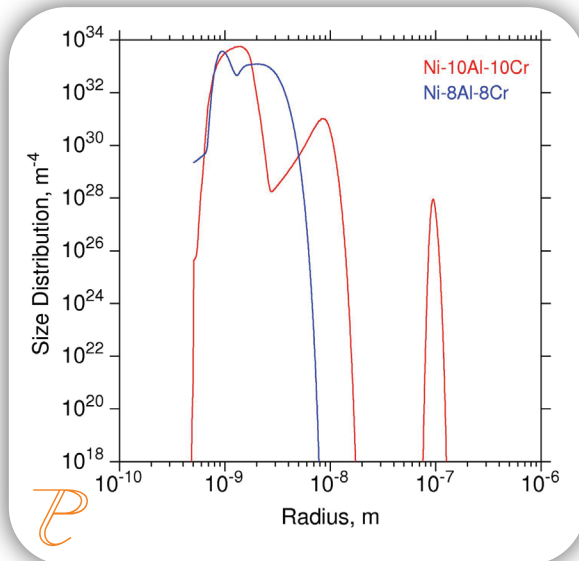
The TTT diagram on the right shows the start of $M_{23}C_6$ precipitation in a 308 stainless steel composition.



Calculate precipitate size distributions

The Precipitation Module can also simulate specific heat treatment schedules under both isothermal and non-isothermal conditions. This enables the prediction of particle size distributions of precipitate phases, as well as number density, mean radius, volume fraction, and more.

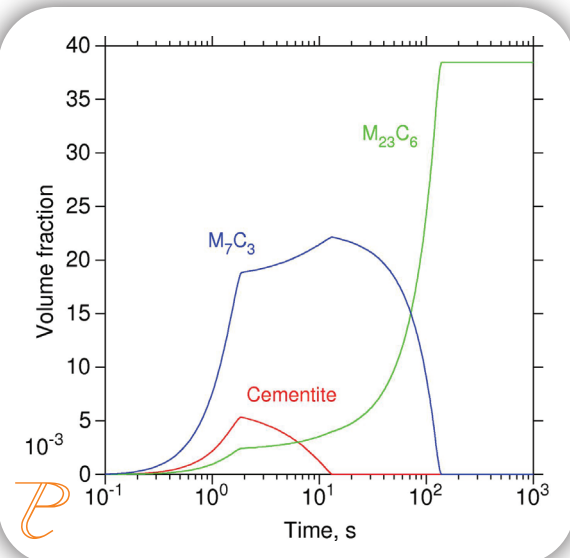
The diagram on the left shows the multi-modal size distribution of γ' during non-isothermal treatment of a Ni-Based superalloy.



Predict stable/metastable precipitation

Many alloys rely on metastable phases for precipitate strengthening. The competition between stable and meta-stable phases is sensitive to the temperature history and alloy chemistry.

In the example on the right, a heat treatment is simulated for a martensitic stainless steel. M_7C_3 and Cementite initially nucleate and grow, but at longer times, these dissolve in favor of the more thermodynamically stable $M_{23}C_6$ carbide. At even longer times, the $M_{23}C_6$ carbide reaches its equilibrium volume fraction and begins to coarsen, which can also be simulated with the precipitation module.



Surface Hardening

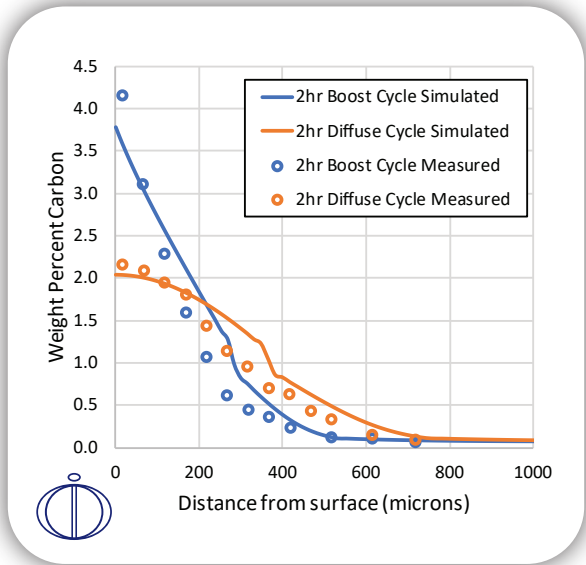
Calculating furnace activities based on gas ratios

Thermo-Calc is not just for alloys and can be used to calculate critical activities and partial pressures for complex furnace gas mixtures at temperature.

The table on the right highlights some different potentials that heat treaters need to control for a nitriding/nitrocarburizing treatment. Each of these partial pressures, potentials and activities can be directly calculated from Thermo-Calc.

Activity to potential	Partial Pressure	Process
$a_N = K_1 * K_N$	$K_N = p_{NH_3}/p^{1.5}H_2$	Nitriding
$a_C = K_2 * K_{CB}$	$K_N = p_{2CO}/p_{CO_2}$	Nitro-carburizing
$a_C = K_3 * K_{CW}$	$K_N = p_{H_2} * p_{CO}/p_{H_2O}$	
$a_C = K_4 * K_{C-O_2}$	$K_N = p_{H_2}/p_{H_2O}$	
$a_C = K_5 * K_{C-CH_4}$	$K_N = p_{CH_4}/p^{0.5}O_2$	Oxi-nitriding / postoxidizing
$a_N = K_6 * K_N$	$K_N = p_{H_2O}/p_{H_2}$	

Reproduced from: Winter, K-M., Torok, P., Industrial Heating, Sep 2010, pp. 61-68.



Predict carburization depth profiles

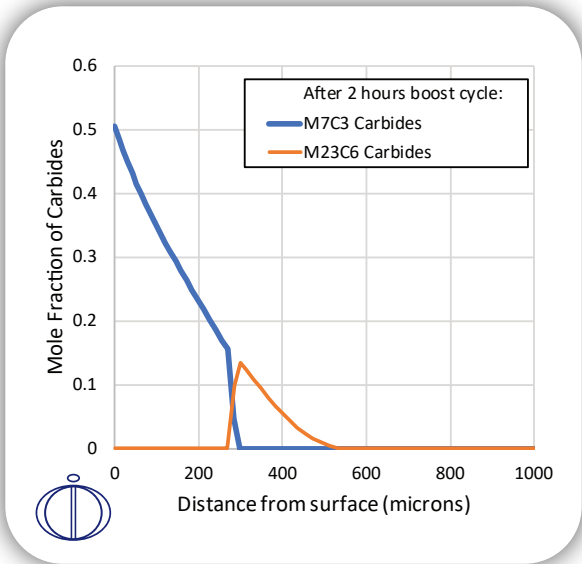
The Diffusion Module can be used to predict diffusion of elements in a phase as a function of chemistry, temperature, time and distance for isothermal and non-isothermal conditions.

In the example on the left, the case depth of carbon diffusing into a highly alloyed steel can be predicted as a function of distance and time, for both boost and diffuse cycles.

The boundary condition can be fixed to a specific activity of carbon in the furnace, or it can be set to a flux which takes into account mass transport.

Determine type and amount of carbides

As carbon diffuses into the alloy during the boost cycle, the concentration builds up near the surface as it cannot diffuse into the alloy fast enough. As carbon supersaturates, precipitate phases form, such as M_7C_3 and $M_{23}C_6$. This can be predicted using Thermo-Calc as can the time required to dissolve these precipitates during the diffuse cycle. The volume fraction of carbides vs. distance is shown for the same simulation above after the 2 hour boost cycle.

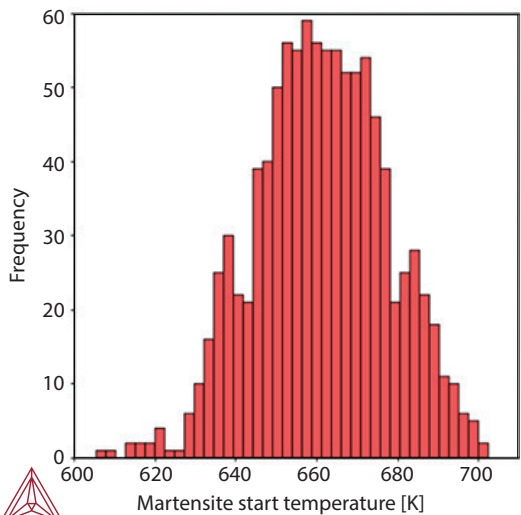
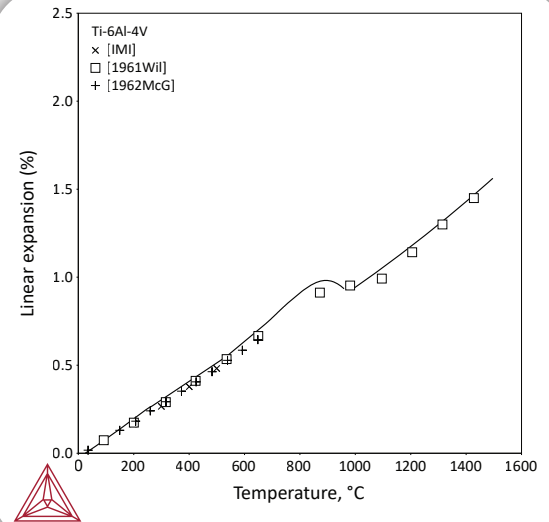


Stress Relief and Quenching Treatments

Generate thermophysical data

Finite element codes are typically used to model thermal stresses. These codes rely on good materials data to make accurate predictions. Handbooks typically only have data for the most common alloys. What do you do when you don't have the data for your alloy, or it doesn't exist?

Thermo-Calc can be used to predict thermophysical properties for multicomponent alloys as a function of chemistry and temperature, such as specific heat, enthalpy, density and liquid viscosity. The calculation on the right shows the linear expansion vs. temperature for a Ti-6Al-4V alloy.



Property variation across alloy specifications

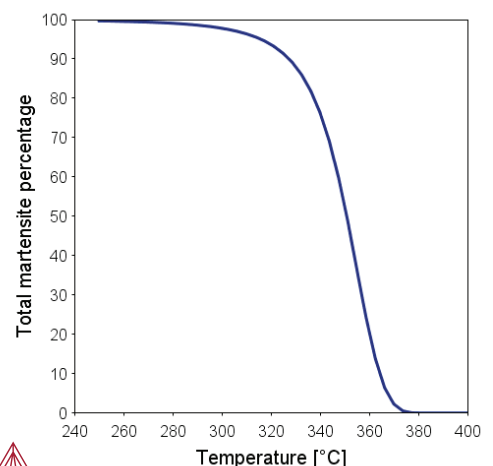
Properties vary both with temperature but also composition. Handbooks or experiments may establish a value for a nominal composition but how that property may vary with chemistry over the material specification range can still be unknown. Thermo-Calc allows you to predict what kind of variation may be expected due to chemistry changes alone.

The figure on the left shows the calculated Ms temperature variation across the 410 stainless steel composition specification. The Ms temperature for a commercial heat has been found experimentally to be 672K by Stone (Thesis: Ohio State University, 2017).

Calculate martensite fractions vs temperature

The Steel Property Model Library available for Thermo-Calc enables the prediction of martensite start temperatures and martensite fraction as a function of temperature. Pearlite growth during heat treatment can also be simulated.

The diagram on the right shows the martensite fractions as a function of temperature for a 4130 steel.



Software and Databases



Thermo-Calc

Software for calculating thermodynamic properties and phase equilibria, including:

- ✓ Stable and metastable equilibrium
- ✓ Amount and composition of phases
- ✓ Transformation temps (liquidus, solidus, A1, A3, solvus, etc.)
- ✓ Density/Thermal expansion
- ✓ Solidification segregation
- ✓ Enthalpy, heat capacity, latent heat
- ✓ Activities and partition coefficients
- ✓ Phase diagrams



Diffusion Module (DICTRA)

Add-on module for simulating diffusion and diffusion controlled transformations, including:

- ✓ Carburizing, decarburizing, nitriding, and carbonitriding
- ✓ Microsegregation during solidification
- ✓ Homogenization treatment
- ✓ Precipitate growth and dissolution
- ✓ Precipitate coarsening
- ✓ Interdiffusion in coating/substrate systems
- ✓ TLP bonding of alloys (brazing)



Precipitation Module (TC-PRISMA)

Add-on module for simulating precipitation kinetics, including:

- ✓ Particle Size Distribution
- ✓ Number Density
- ✓ Average Particle Radius
- ✓ Volume Fraction
- ✓ TTT/CCT
- ✓ Average Compositions
- ✓ Interface Compositions
- ✓ Nucleation Rate
- ✓ Critical Radius

Thermodynamic, Properties, and Mobility Databases

The quality of the predictions in Thermo-Calc are strongly dependent on the database. We employ a highly qualified team to ensure that our databases are up-to-date and of the highest quality. An extensive selection of thermodynamic, properties, and mobility databases are available, including, but not limited to:

Steels and Fe-alloys	Cu-based alloys	Aqueous Solutions	Ceramics
Ni-based superalloys	High Entropy alloys	Nuclear Materials	Semi-conductors
Al-based alloys	Si-based alloys	Geochemical	Super-conductors
Ti-based alloys	Solders	Slags	Gases
Mg-based alloys	Molten Salts	Noble metals	TBC, SOFC

Predictions are Based on Scientifically Supported Data and Models

Thermo-Calc is based on the CALPHAD Methodology:

- Self-consistent approach to thermodynamics and phase equilibria
- Captures composition and temperature dependence
- Assessment of binary and ternary subsystems allows extrapolation into multi-component space
- Databases for a wide range of material systems and applications
- Methodology extended into diffusion, precipitation, and other material property models

$$G(p, T) = H - TS$$

Gibbs Free Energy

$$\frac{\partial \varphi}{\partial t} = D \frac{\partial^2 \varphi}{\partial x^2}$$

Ficks Laws of Diffusion

$$\Delta G = \frac{4}{3}\pi r^3 \Delta g + 4\pi r^2 \sigma$$

Classical Nucleation Theory

*Empowering metallurgists, process engineers
and researchers to make better decisions*

18000+ journal citations from customers

1000+ citations in patents

40+ year track record

1600+ organizations

60+ countries

About Thermo-Calc Software

Thermo-Calc Software is a growing company that specializes in developing software for computational materials engineering. Our software products are used for both fundamental and applied research, such as design of new alloys, optimization of processing conditions, trouble shooting and much more.