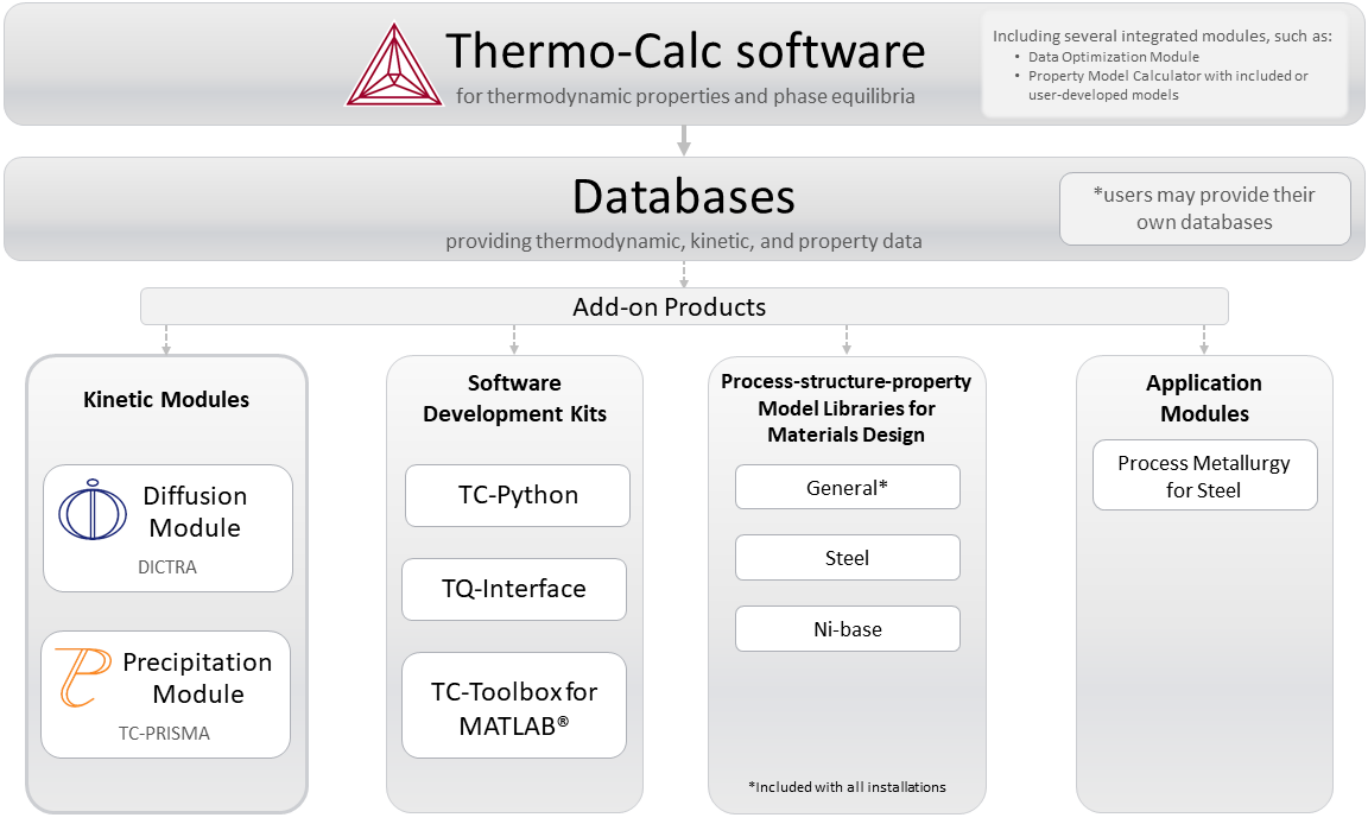
Thermo-Calc News
2022a release

Anders Engström

Thermo-Calc Software, Stockholm, Sweden

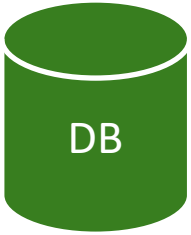
December 17th, 2021

Product overview



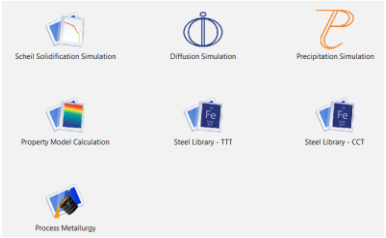
Focus in our development is on:

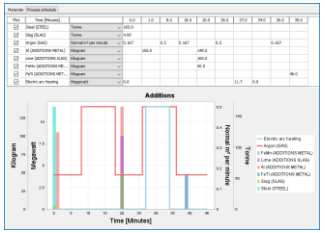
- ❑ User experience
- ❑ Data relevance/quality
- ❑ Functionality
- ❑ Interoperability

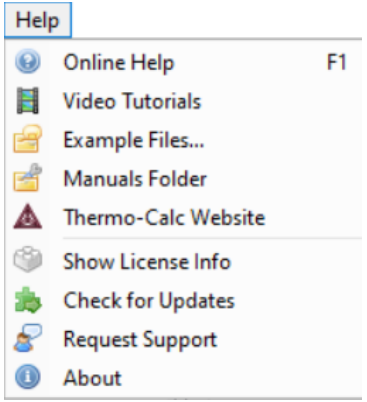


User experience - past 5 years

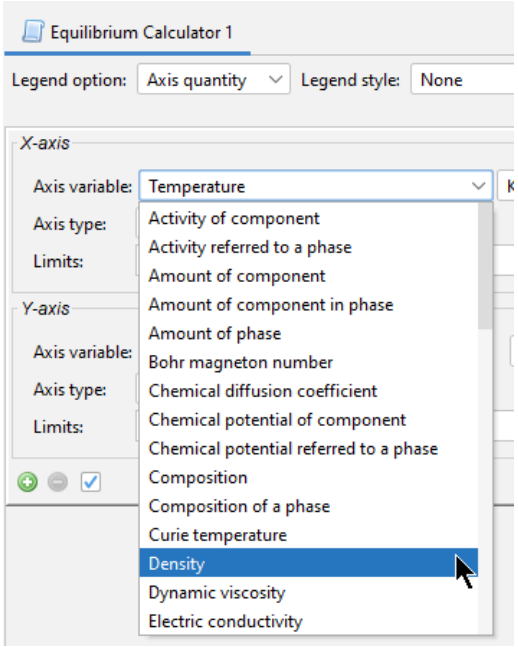
- ❑ Precipitation Module (TC-PRISMA) integrated into Thermo-Calc framework
- ❑ Diffusion Module (DICTRA) available in Graphical Mode
- ❑ Process Metallurgy Module introduced, for easy calculation of liquid metal / slag eq. & simulation of e.g. AOD/ladle furnace using the EERZ model
- ❑ On-line help
- ❑ Continuous improvements to documentation
- ❑ New examples
- ❑ New video tutorials







User experience - introduced with 2022a



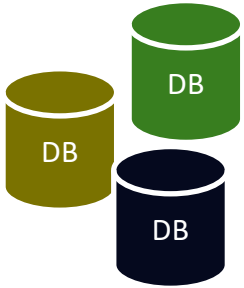
- Several Quantities Now directly Available for Plotting and Tabulating Instead of Entering as a Function, e.g. ***Volume fraction of phase, Density, Heat Capacity,….***
- 4 New Examples
- New video tutorials
- **A self-paced learning hub** has been developed and is available from our website on a subscription basis.

Data relevance and quality - past 5 years

Thermo-Calc Software

Several new and/or updated Databases made available, e.g.:

- **New databases** introduced in the period, e.g.
  - High-Entropy Alloys (TCHEA, MOBHEA)
  - Copper alloys (TCCU, MOBCU)
  - Ti- and TiAl-alloys (TCTI, MOBTI)
  - Precious alloys (TCNOBL)
  - Solder alloys (MOBSLD)



- **Updates and/or revisions** of all major databases, e.g.
  - TCFE
  - TCNI
  - TCOX
  - TCAL
  - TCMG
  - TCHEA
  - TCCU
  - TCTI
  - TCSLD

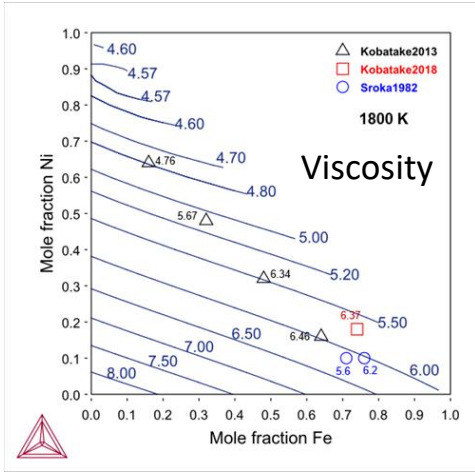
- Other updates include, e.g.
  - MEPH19, NUCL19, SSUB6

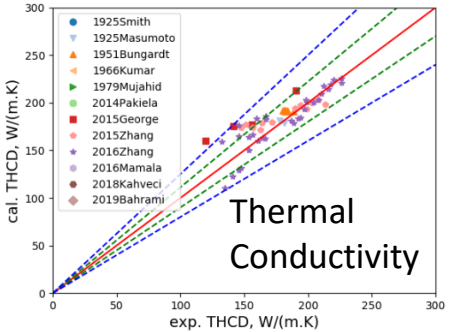
Data relevance and quality - past 5 years

Thermo-Calc Software

Several new properties modelled, e.g.:

- **Molar volume** (in general) included in most databases
- **Volume of slag and metallic liquid** added to:
  - Oxides and Slags (TCOX)
- **Viscosity & Surface tension of liquid** added to:
  - Steel an Fe-based alloys (TCFE)
  - Nickel-based alloys (TCNI)
  - Aluminium alloys (TCAL)
  - Magnesium alloys (TCMG)
  - Copper Alloys (TCCU)
  - Ti/TIAl-alloys (TCTI)
  - High-Entropy Alloys (TCHEA)
  - Solder alloys (TCSLD)
  - Oxides and Slags (TCOX)
- **Thermal conductivity / Electric resistivity** added to:
  - Nickel-based alloys (TCNI)
  - Aluminium alloys (TCAL)
  - Magnesium alloys (TCMG)
  - High-Entropy Alloys (TCHEA)





Data relevance and quality - introduced with 2022a

Thermo-Calc Software

New Databases:

- ❑ TCS Permanent Magnetic Materials Database (TCPMAG1)
- ❑ TCS Zr-based Alloys Database (TCZR1)
- ❑ TCS Noble Metal Alloys Mobility Database (MOBNOBL1)

New versions of thermodynamic and kinetic databases:

- ❑ TCS Steel and Fe-alloys Database (TCFE12)
- ❑ TCS Steels/Fe-Alloys Mobility Database (MOBFE7)
- ❑ TCS Ti/TiAl-based Alloys Database (TCTI4)
- ❑ SGTE Solutions Database (SSOL8)
- ❑ TCS Al-alloys Mobility Database (MOBAL7)

Updates to:

- ❑ TCS Mg-based Alloys Database (TCMG6.2)
- ❑ TCS Al-based Alloys Database (TCAL8.1)
- ❑ TCS Solder Alloy Solutions Database (TCSLD4.1)
- ❑ TCS High Entropy Alloys Database (TCHEA5.1)
- ❑ TCS Metal Oxide Solutions Database (TCOX10.2 and 11.1)
- ❑ TCS Ni-based Superalloys Database (TCNI11.0.1)

Data relevance and quality - introduced with 2022a

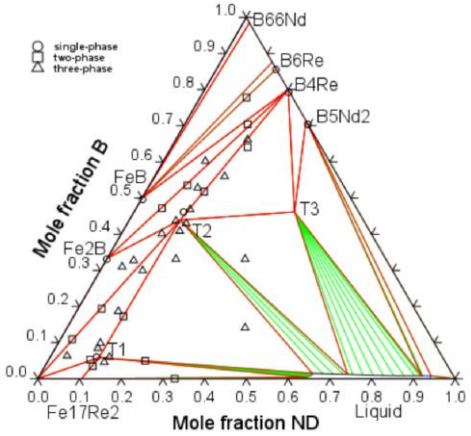
TCS Permanent Magnetic Materials Database (TCPMAG1)

This new database was developed for the NdFeB based permanent magnets.

- 6 elements are included: **B, Ce, Fe, La, Nd, Pr**
- All 15 binary systems assessed
- 11 ternary systems are assessed based on the published experimental data

B-Ce-Fe	B-Ce-Nd	B-Fe-La	B-Fe-Nd	B-Fe-Pr	Ce-Fe-La
Ce-Fe-Nd	Ce-Fe-Pr	Ce-La-Pr	Fe-La-Nd	Fe-Nd-Pr	

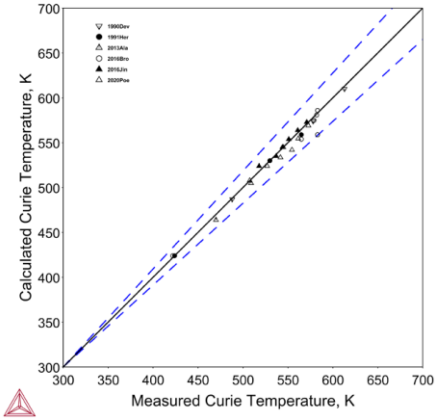
- 19 phases are included



Fe-Nd-B isothermal section at 1173K

Thermophysical Properties

- Molar Volume of liquid & solid phases
- Viscosity of liquid
- Surface tension of liquid



Curie Temperatures for the T1 phase: (Nd,La,Ce,Pr)2Fe14B

In all cases the differences are less than 5%.

Data relevance and quality - introduced with 2022a

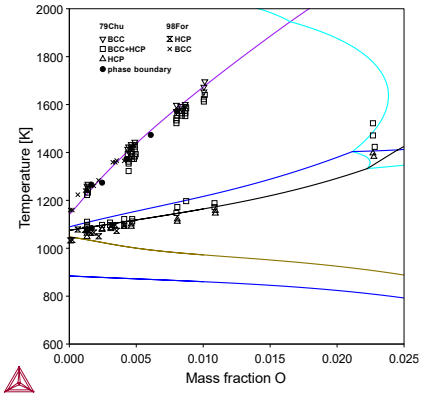
TCS Zr-based Alloys Database (TCZR1)

This new database can be used for a wide range of compositions from pure zirconium to complex zirconium-based commercial zirconium alloys.

- 8 elements are included: **Cr, Fe, H, Nb, Ni, O, Sn, Zr**
- All 28 binary systems are assessed for their full range of composition
- 19 ternary systems including all Zr-containing ternaries that has published experimental data together with many ternary systems for the major alloying elements are assessed

Cr-Fe-Nb	Cr-Fe-Sn	Cr-Fe-Zr	Cr-Nb-Sn	Cr-Nb-Zr	Cr-Ni-Zr
Cr-O-Zr	Cr-Sn-Zr	Fe-Nb-Ni	Fe-Nb-Zr	Fe-Ni-Zr	Fe-O-Zr
Fe-Sn-Zr	H-Nb-Zr	Nb-Ni-Zr	Nb-O-Zr	Nb-Sn-Zr	Ni-O-Zr
Ni-Sn-Zr					

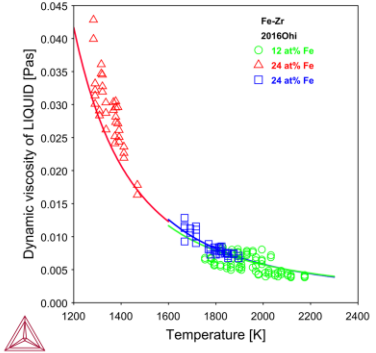
- 69 phases are included



Calculated phase boundaries of the pseudobinary Zircaloy 2/4-system

Thermophysical Properties

- Molar Volume of liquid & solid phases
- Viscosity of liquid
- Surface tension of liquid



Dynamic Viscosity of Fe-Zr Alloys

Data relevance and quality - introduced with 2022a

Thermo-Calc Software

TCS Steel and Fe-alloys Database (TCFE12)

- New thermophysical properties:
  - **Thermal conductivity**
  - **Electrical resistivity**

- Added **Tin (Sn)**:
  - **26 Binaries** Sn-X (X=Al, B, C, Ca, Ce, Co, Cr, Cu, Fe, Mg, Mn, Mo, Nb, Ni, O, P, Ru, S, Si, Sn, Ta, Ti, V, W, Y, Zn, Zr)
  - **13 Ternaries**: Fe-Sn-X (X=C, Cr, Cu, Mn, Nb, Ni, O, S, Si, W, Zn, Zr), and Al-C-Sn

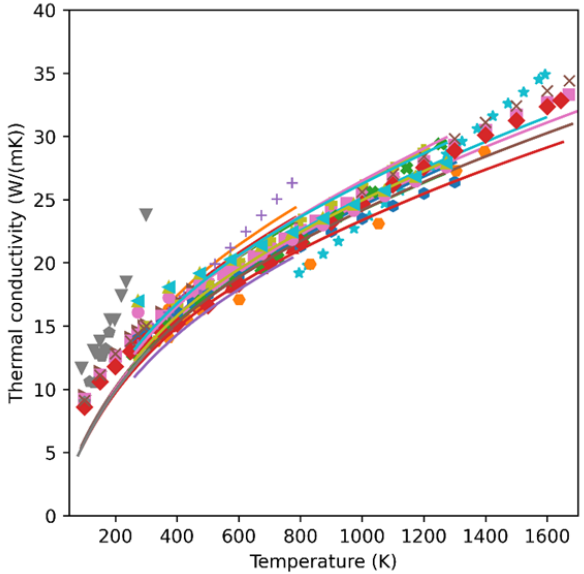
- Updated **Zinc corner**, as well as systems related for the **galvanization** process:
  - Remodelled and unified all gamma-brass D82 phases stable in Fe-Zn, Cu-Zn, Ni-Zn, Mn-Zn, Co-Zn with a 4SL **FE3ZN7_D82**.
  - Added **8 Ternaries:** Al-Fe-Mg, Cu-Fe-Zn, Fe-Ni-Zn, Fe-Si-Zn, Fe-Mg-Si, Fe-Mg-Ni, Fe-Mn-Zn, Mg-Si-Zn

- Several other updates

Data relevance and quality - introduced with 2022a

TCS Steel and Fe-alloys Database (TCFE12)

Thermal conductivity of **Cr-Ni austenitic stainless steel alloys**.

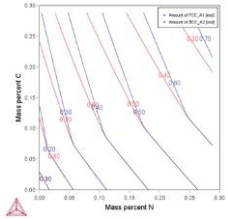


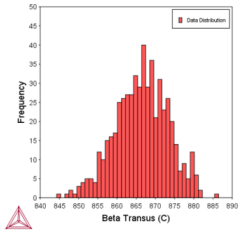
- Fe-18.5Cr-9.21Ni-0.19Mn-0.11C
- Fe-19.6Cr-8.96Ni-0.37Mn-0.24C
- Fe-19.6Cr-7.99Ni-0.28Mn-0.24C
- Fe-18.08Cr-9.12Ni-0.59Mn-0.47Si-0.34Ti-0.07C-0.013P-0.003S
- Fe-18Cr-9Ni-2Mn-1Si-0.15C-0.045P-0.03S
- Fe-19Cr-9.25Ni-2Mn-1Si-0.08C-0.045P-0.03S
- Fe-19Cr-9.25Ni-2Mn-1Si-0.08C-0.045P-0.03S
- Fe-18.49Cr-8.61Ni-1.69Mn-0.4Si-0.21Cu-0.21Mo-0.12Co-0.051C-0.029S
- Fe-18.72Cr-9.98Ni-1.31Mn-0.7Si-0.09Mo-0.05Cu-0.041P-0.026C-0.012S
- Fe-20Cr-11Ni-2Mn-1Si-0.08C-0.045P-0.03S
- Fe-17Cr-12Ni-2.5Mo-2Mn-1Si-0.08C-0.045P-0.03S
- Fe-17.45Cr-12.6Ni-2.55Mo-1.59Mn-0.6Si-0.19Co-0.09Cu-0.063C-0.023P-0.01S
- Fe-17Cr-12Ni-2.5Mo-2Mn-1Si-0.045P-0.03C-0.03S
- Fe-17.4Cr-12.3Ni-2.5Mo-1.8Mn-0.46Si-0.2Cu-0.17Co-0.06N-0.027P-0.024C-0.01Nb-0.008B-0.002S
- Fe-18Cr-10.5Ni-2Mn-1Si-0.08C-0.045P-0.03S
- Fe-19.58Cr-11.95Ni-1.24Mn-0.032C-0.008P-0.008S-0.004Al
- Fe-18.55Cr-11.5Ni-1.3Mn-0.7Si-0.07Mo-0.04C-0.016N
- Fe-17.69Cr-11.09Ni-1.26Mn-0.53Si-0.33Mo-0.12Cu-0.03C-0.027P-0.017S
- Fe-17.25Cr-8.3Ni-1.22Mn-0.37Si-0.084C-0.019P-0.01S

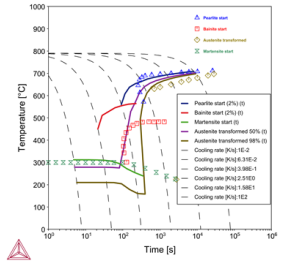
The values are calculated by freezing-in the state at the typical annealing temperature of manufacture for each alloy.

[1991Madelung] O. Madelung, G.K. White, eds., Metals: Electronic Transport Phenomena – Thermal Conductivity of Pure Metals and Alloys, in: Therm. Conduct. Pure Met. Alloy., Springer-Verlag, Berlin/Heidelberg, 1991.

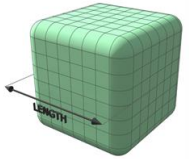
Functionality - past 5 years



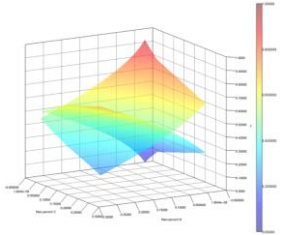




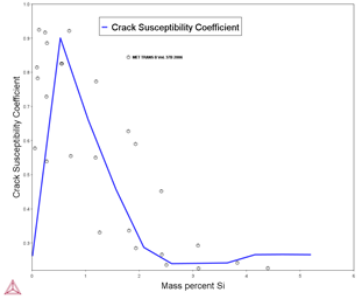
- Property Model Calculator
- Uncertainty prediction
- Property model library for Steel and calculation of TTT/CCT-diagrams
- Possibility to enter an initial size distribution in Precipitation Module (TC-PRISMA)
- Non-spherical morphologies in Precipitation Module (TC-PRISMA)



- NPLE and Para-equilibrium growth models in Precipitation Module (TC-PRISMA)



- 3D-plots for grid calculations

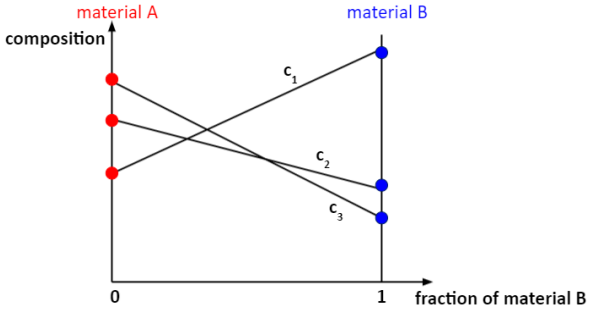


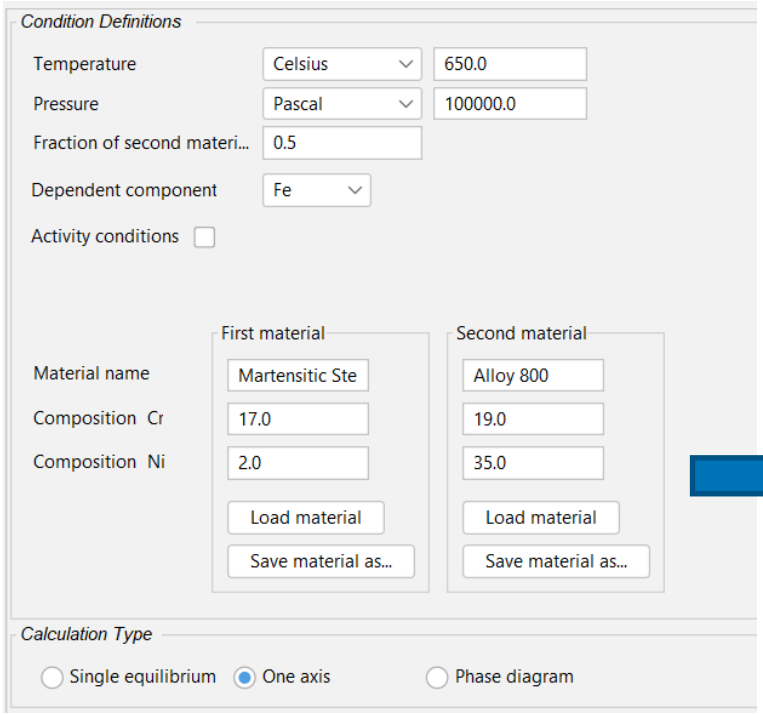
- Extension of Scheil-module to account for back-diffusion and solute trapping
- Several new property models introduced, e.g. yield strength, crack susceptibility,….

Functionality - introduced with 2022a

Thermo-Calc Software

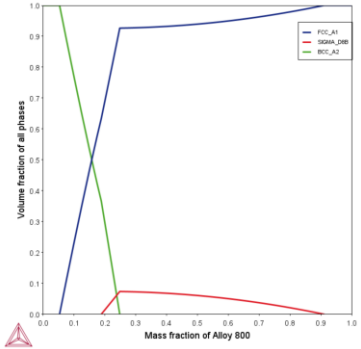
- Material to Material calculator, i.e. step and map calculation between an alloy A and B.





Typical applications include:

- **Graded materials** produced by e.g. additive manufacturing
- **Non-similar material joints**, such as welds of Ti with Ni-alloy
- **Reaction of two materials**, for instance, the influence of volcanic ash on a turbine component in an engine



Functionality - introduced with 2022a

- Models for grain growth and particle (Zener) pinning in Precipitation Module (TC-PRISMA).

Matrix Phase

Phase: BCC_A2 — Hide details

Elastic properties: Disregard

Molar volume: Database 7.0E-6 m^3/mol

Grain growth: ☑

Grain size: Edit grain size distribution

Grain boundary energy: 0.5 J/m^2

Grain boundary mobility: Prefactor: 0.004 m^4/Js Activation energy: 242000.0 J/mol

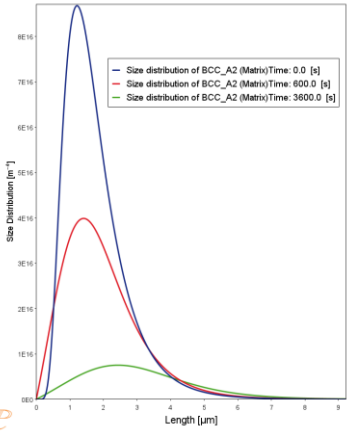
Grain aspect ratio: 1.0

Zener pinning: ☑

Dislocation density: 5.0E12 m^{-2}

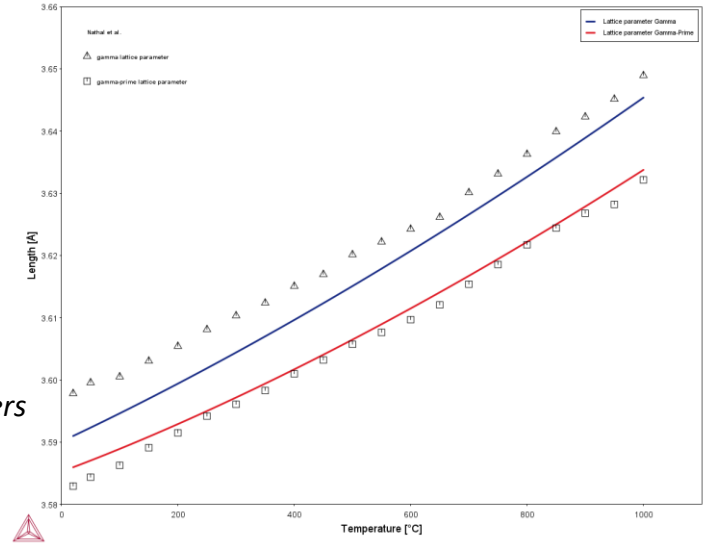
Deformation strain: 1.0

Mobility enhancement: Prefactor: 1.0 Activation energy: 0.0 J/mol

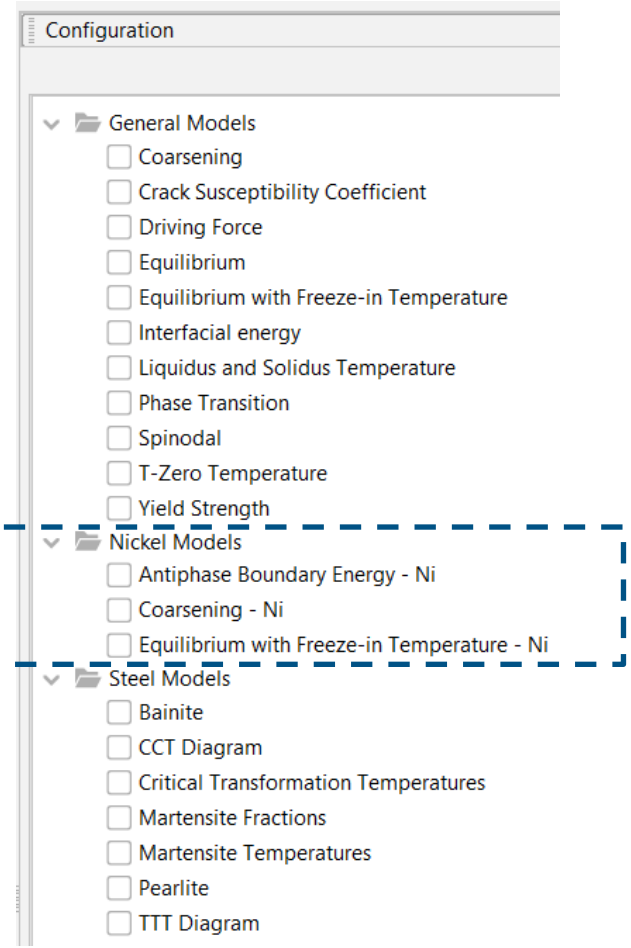


Functionality - introduced with 2022a

- Property model library for Ni-alloys, including models for:
  - Anti Phase Boundary (APB) Energy
  - Coarsening kinetics,
  - Equilibrium with Freeze-in Temperature

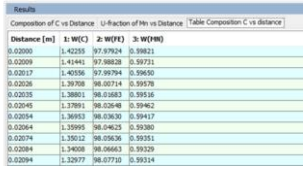


Calculated lattice parameters for γ and γ' in NASAIR 100

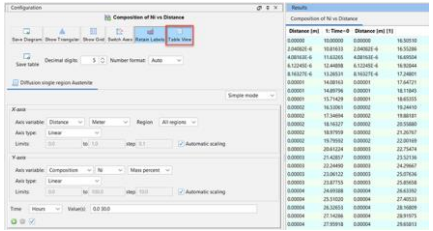


Interoperability - past 5 years

- Tabulation of Results



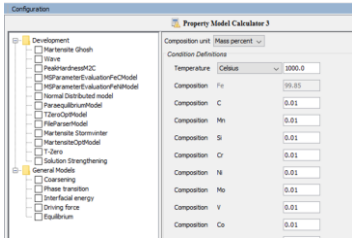
- Converting Plot to Table data



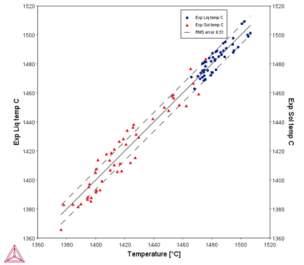
- TC-Python

- New TC-Toolbox for MATLAB® with Extensive Functionality

- Property Model Development Framework



- Batch Calculations type for High Throughput Calculations



Interoperability - introduced with 2022a

Thermo-Calc Software

- Several minor improvements and bug fixes to TC-Python and TC-Toolbox for MATLAB®

  - SDK-905 TC-Python auto-complete broken in PyCharm of versions later than 2020.3.5. This has now been fixed
  - SDK-776 The possibility to get interfacial_energy from a SingleEquilibriumCalculation has been added. This is used internally in several property models, but can also be used in any "normal" python scripts using TC-Python.
  - SDK-892: Bookmarked single equilibrium calculation states now also contain the component status (for example "entered", "suspended"), which will now be correctly set when loading a bookmarked state using *set_state_to_bookmark()*.
  - SDK-908 Before Property Models that returned several values did not return anything in case of errors but raised an exception. Now the errors are instead logged, and the corresponding value is set to NaN. That means that the values that are correct in case of errors now are returned.
  - SDK-910: Retrieving result values could fail in TC-Python: In the rare case of having result data with multiple identical values on the x-axis, the `get_values_of` method (and similar) of Scheil, Property Diagram and Phase Diagram result objects could fail with an exception.
  - CMD-914 and CMD-917 The functions for adding and removing dynamic arguments to Property Models is improved. Now you can specify the index of newly created arguments, and as input to the functions you get the index of all previously created arguments.
  - SDK-922 The single equilibrium calculator is now ignoring special elements (i.e., vacancies, positrons, or electrons) defined in the system, when checking if the system elements and defined components are matching.
  - SDK-934 The Property Model SDK is improved regarding how models control visibility of graphical input fields.
  - SDK-946 The method `add_initial_equilibrium` if fixed for phase diagram calculations. Previously there was a problem if it was called before creating the axes.

Thermo-Calc Software

Thank You!

When data matters

www.thermocalc.com