Thermo-Calc Software

Thermo-Calc On-line Training

April 9 - 11 2024

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Thermo-Calc Software

Thermo-Calc Day 1

9:00	S-Eq 1: Stainless steel 2205.
9:30	Introduction to Thermo-Calc and CALPHAD-based software tools.
10:00	S-Eq 2: Ni superalloy CSMX-2.
10:25	Q & A
10:40	S-Eq 3: Stable and metastable phases in Al-Cu.
11:00	Step 1: Ni alloy Nimonic 263.
11:25	Step 2: Slag calculation, changing components.
11:45	Q & A
12:00	Handing out home assignment.

S-Eq = Single-Equilibrium Calculation

Step = One-axis Step Calculation

Schedule

Thermo-Calc Day 2

9:00	About the home assignment.
9:10	Thermodynamic Databases.
9:30	Step 3: Al alloy 6053
9:55	Map 1: Phase diagram for a cemented carbide.
10:25	Q & A
10:40	Map 2: HEA phase diagram.
11:05	Map 3: Phase diagram from base material to weld.
11:40	Q & A
11:55	Handing out home assignment.

Step = One-axis Step Calculation

Map = Phase diagram mapping, 2 axes or more.

Schedule

Thermo-Calc Day 3

9:00	About the home assignment.
9:10	Scheil solidification simulation.
9:40	App1: Alloy design, duplex stainless steel.
10:20	Demo of console mode.
10:30	Q & A
10:45	Property Model Calculation.
11:15	Process Metallurgy Module Calculation.
11:35	Resources for help.
11:45	Q & A
12:00	End.

App = Thermo-Calc calculation applied to a real case.

Download

https://download.thermocalc.com/courses/TC-Day1/

S-Eq1-Stainless2205.tcu	14K
S-Eq2-Ni-alloy-850.tcu	19K
S-Eq3-AlCu-precipitates.tcu	50K
Step1-Nimonic263.tcu	51K
Step2-slag.tcu	31K
TC-Day1.pdf	7.5M

Software Installation

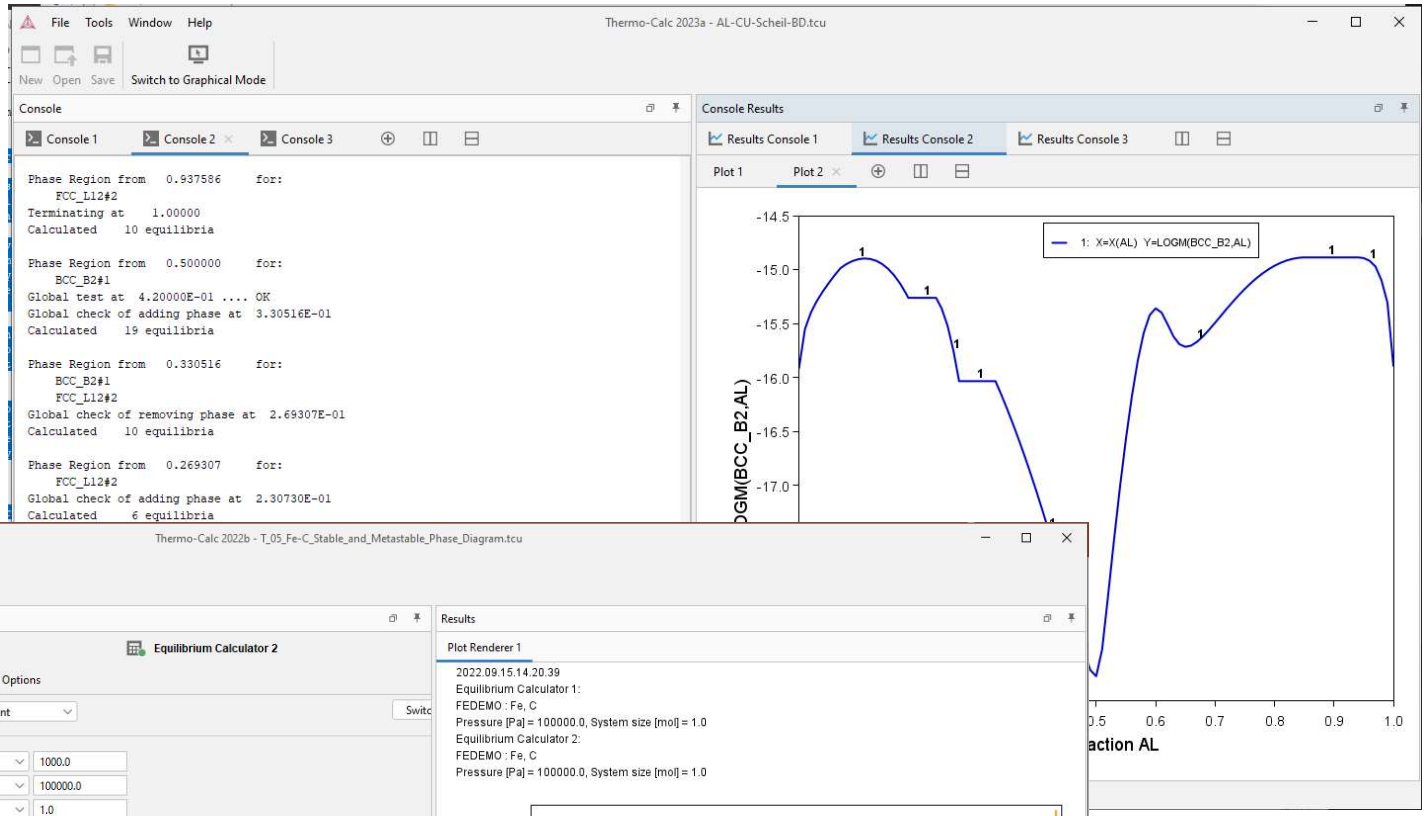
For those of you also joining DICTRA/TC-Prisma:

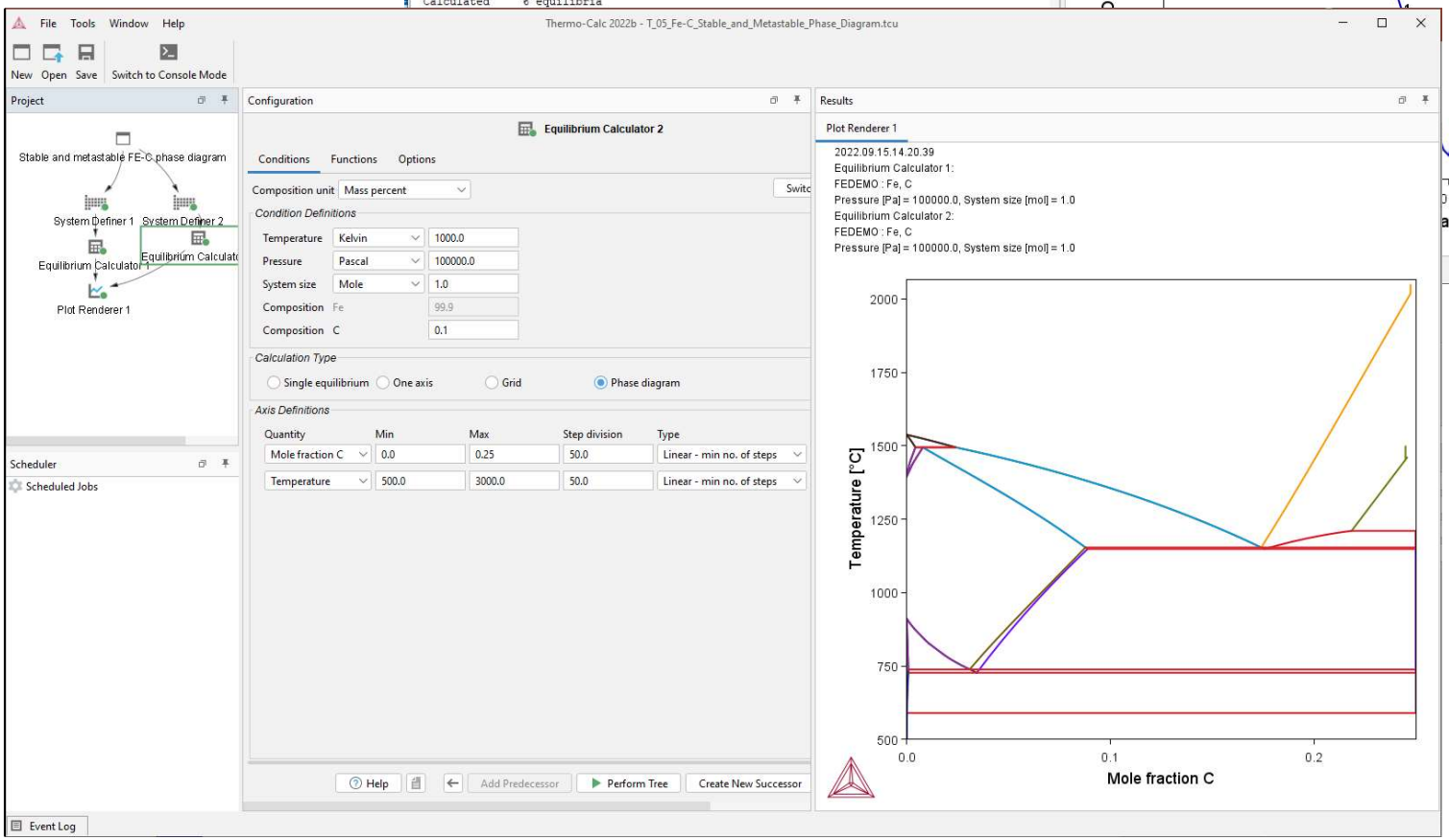
The software installation and license file you have are valid for all software and for the duration of all courses.

Overview of Thermo-Calc 2024a

Thermo-Calc Software

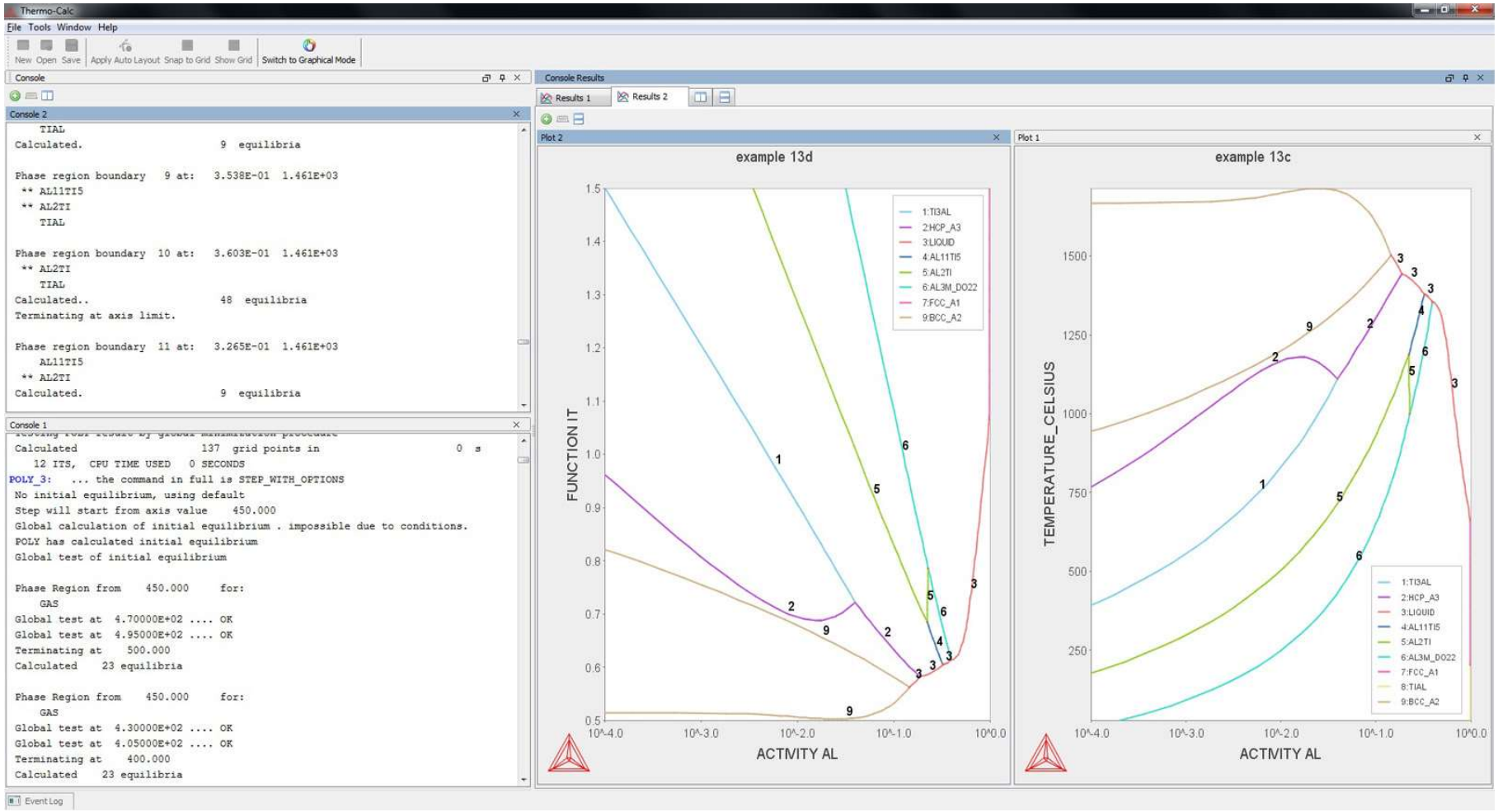
Console Mode



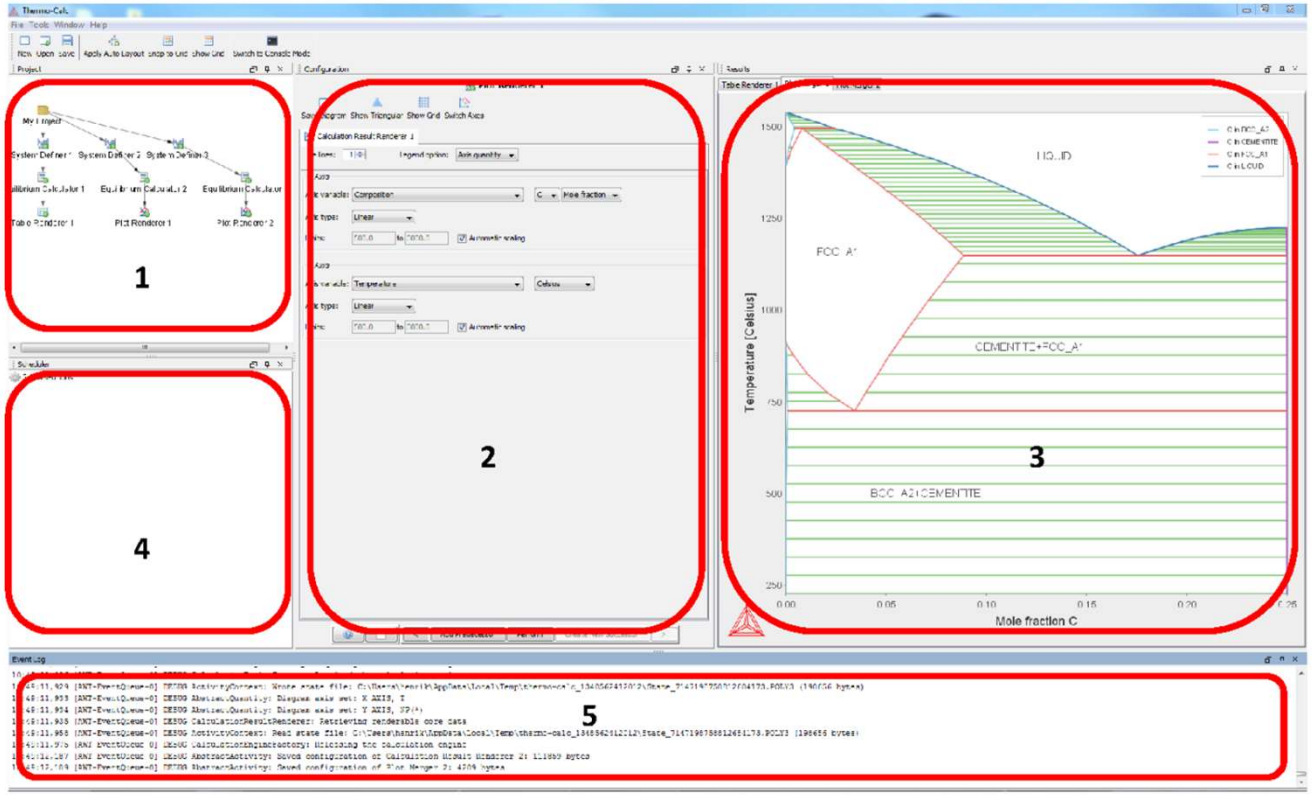


Graphical Mode

Using Console Mode



Graphical mode - GUI Layout

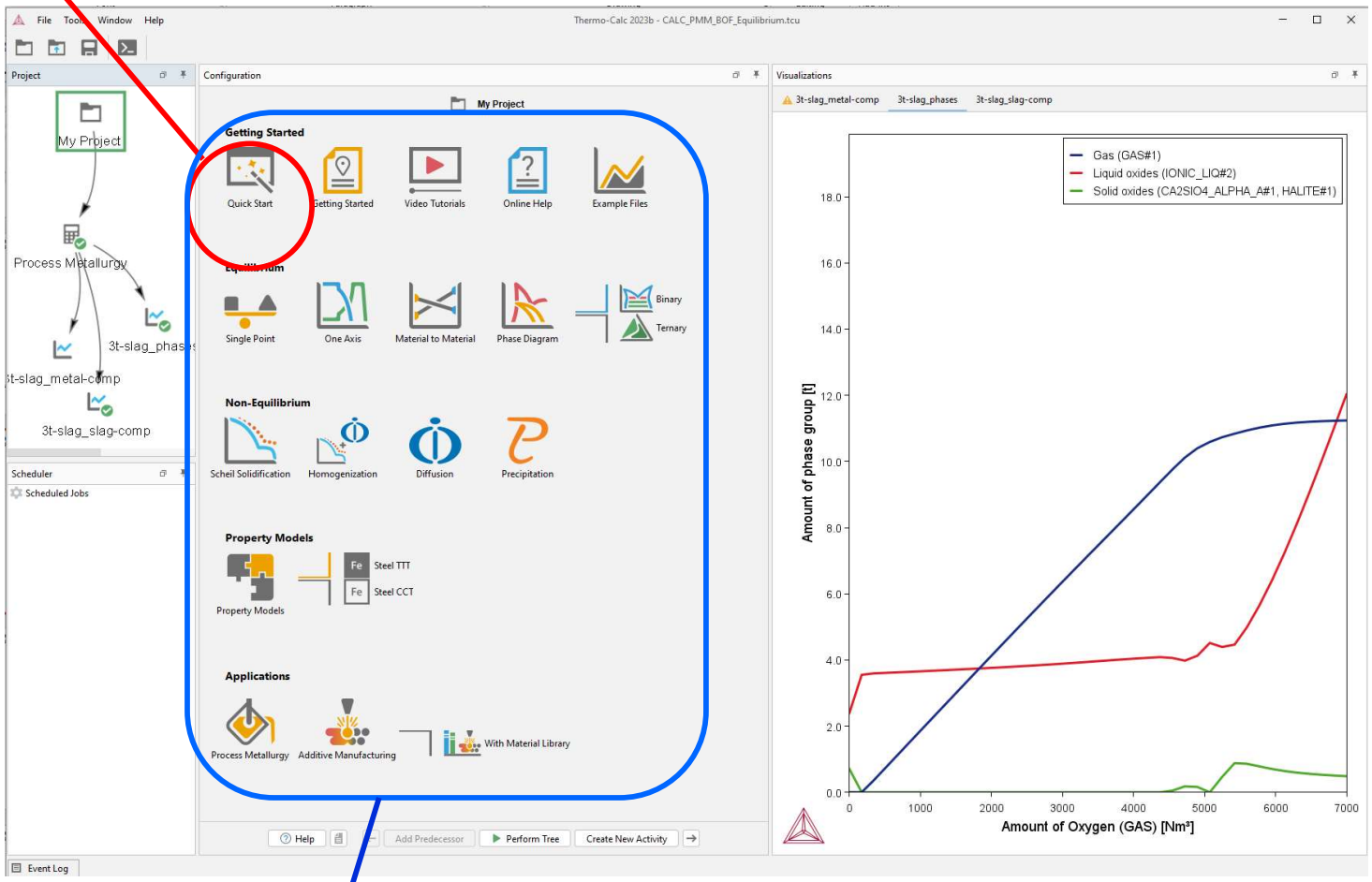


1. Project window – shows relations between defined *activities*
2. Configuration window – for configuring the selected *activity*
3. Results window – graphic and text output
4. Scheduler window – shows performed and scheduled calculations
5. Event log window – text output of progress

Getting Started

”Quick Start”

Step-by-step instructions for some common tasks

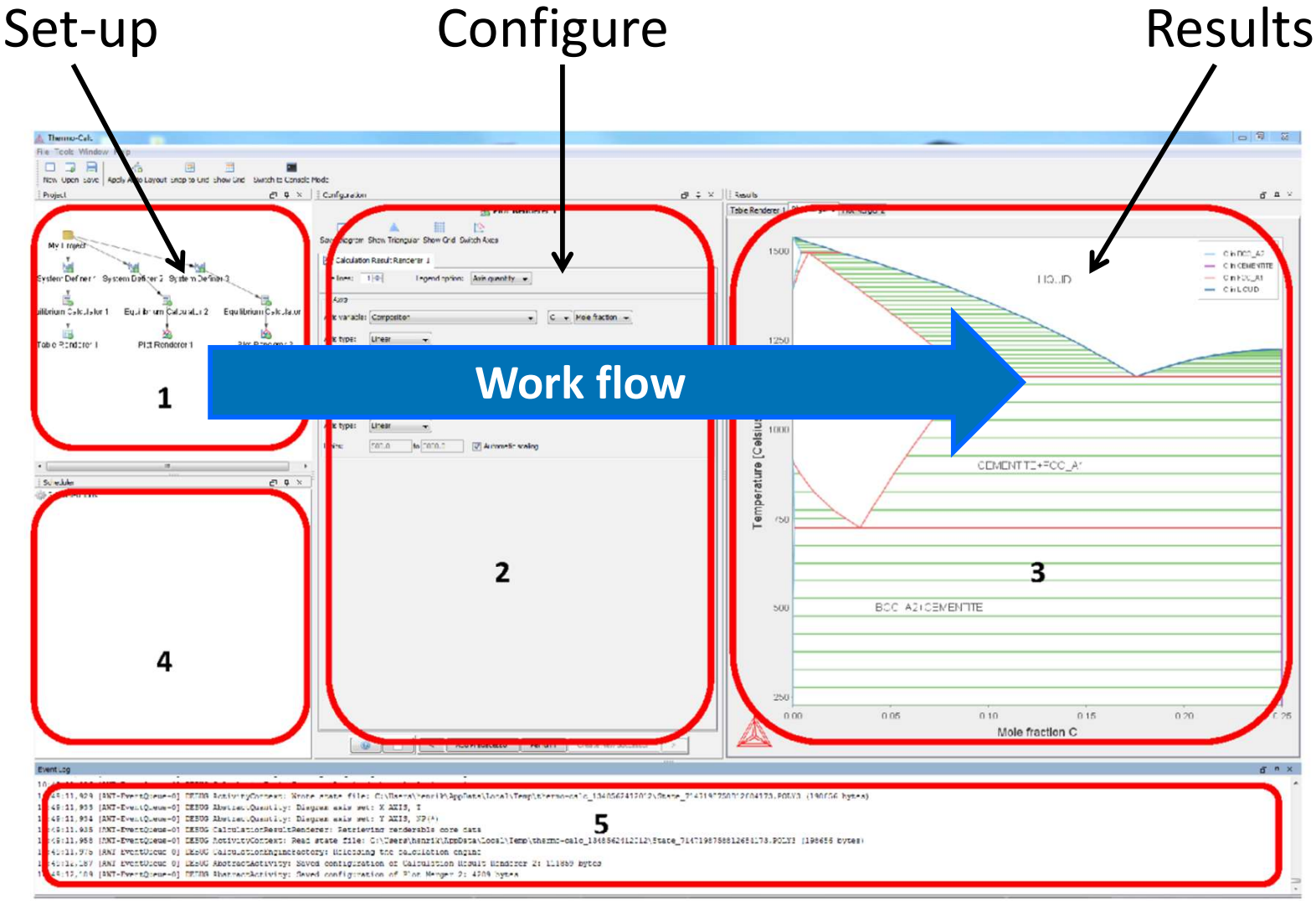


”Templates”

Sets up the framework for certain specific tasks

GUI layout

Thermo-Calc Software



Thermo-Calc Software

Single Point Equilibrium Calculations

Single Equilibrium Calculations

Thermo-Calc Software

Results:

System

Moles	1.00000	
Mass	55.24126	[g]
Temperature	1273.15000	[K]
Total Gibbs Energy	-67901.58065	[J]
Enthalpy	38263.15388	[J]
Volume	7.34999E-6	[m3]

Component	*Mole Fraction*	*Mass Fraction*	*Activity*	*Potential*
Ni	0.10354	0.11000	0.00016	-92477.97589
Cr	0.23373	0.22000	0.00323	-60712.81918
Fe	0.66273	0.67000	0.00185	-66597.42065

Stable Phases

	Moles	*Mass*	*Volume Fraction*	
BCC_A2#1	0.07880	4.31311	0.07968	Composition

Composition

Component	*Mole Fraction*	*Mass Fraction*
Fe	0.61718	0.62968
Cr	0.32829	0.31184
Ni	0.05454	0.05847

	Moles	*Mass*	*Volume Fraction*	
FCC_A1#1	0.92120	50.92814	0.92032	Composition

Composition

Component	*Mole Fraction*	*Mass Fraction*
Fe	0.66663	0.67341
Cr	0.22564	0.21222
Ni	0.10773	0.11436

Thermodynamic Properties:

Gibbs Energy

Enthalpy

Activities

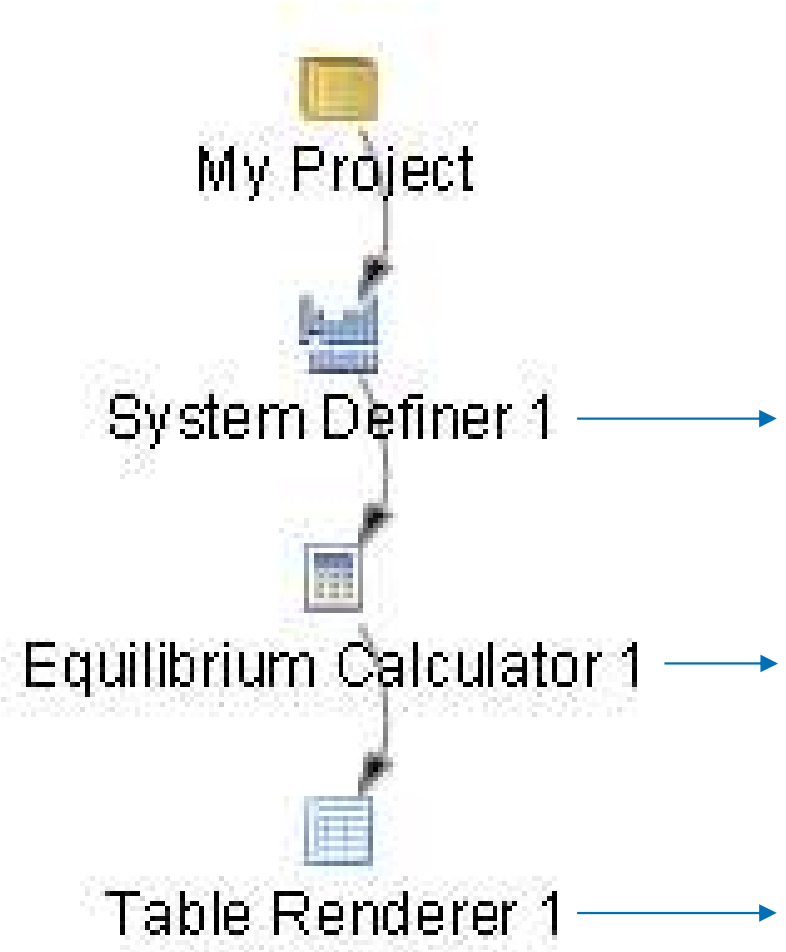
Phase Data:

Equilibrium amounts

Equilibrium compositions

The results are viewed in the Table Renderer.

General work flow



Select database
Define the thermodynamic system

Set equilibrium conditions

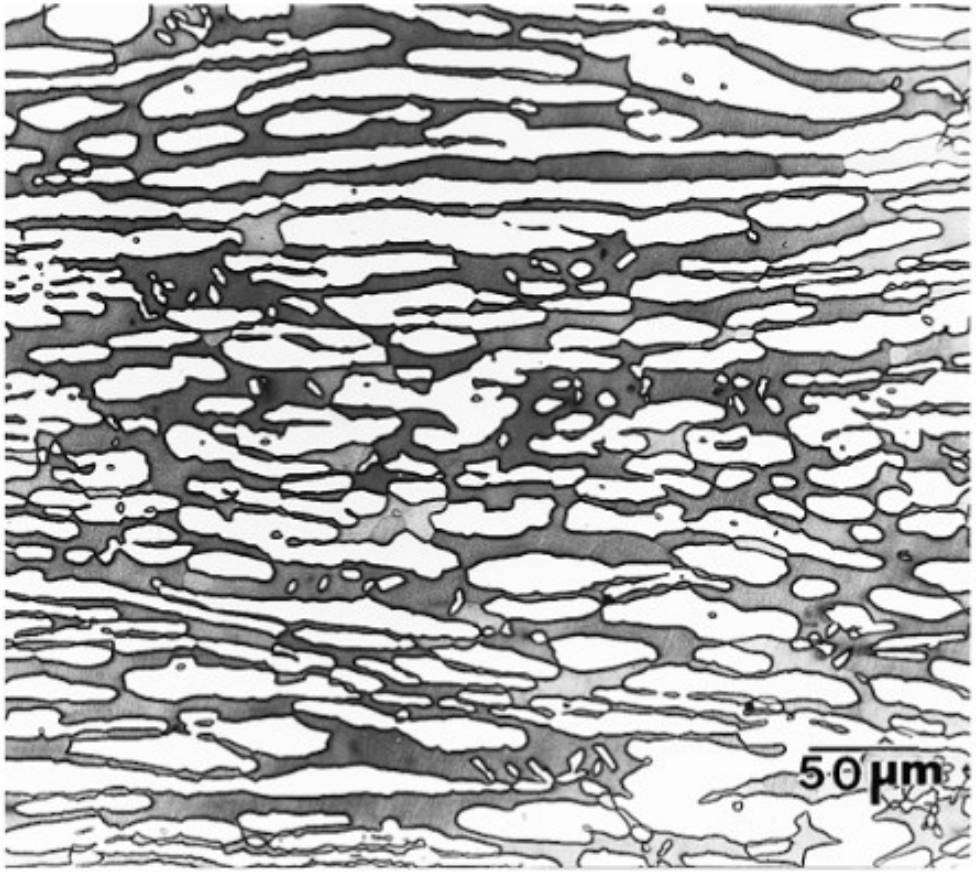
View results

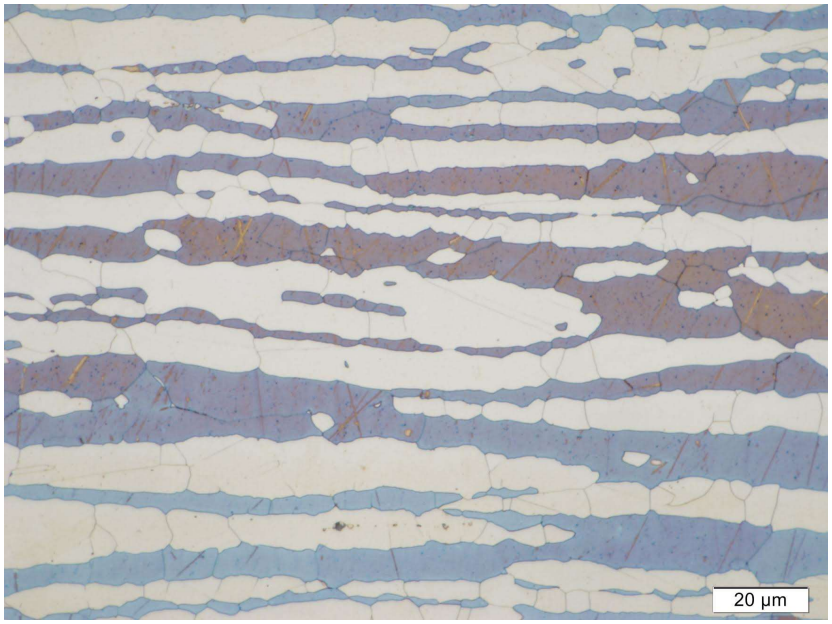
S-Eq 1: Heat treatment of duplex stainless steel 2205 at 1050 °C.

Single Equilibrium, Example 1

Duplex 2205 – Fe - 22Cr – 5 Ni – 0.02C – 1.8Mn – 2.5Mo – 0.1N (wt-%)

Temperature: 1050°C (typical solution annealing temp)



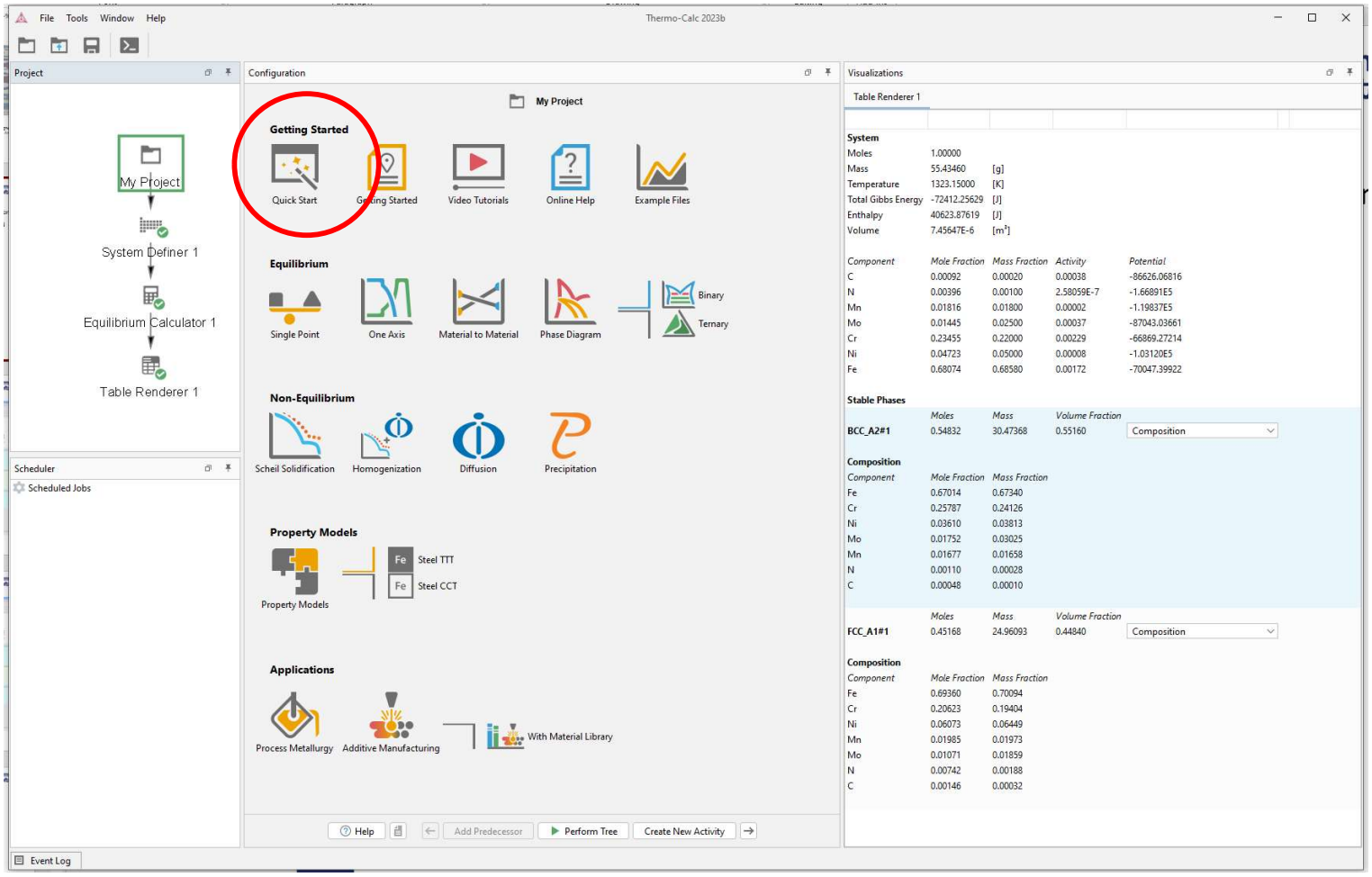


Bramfitt, Bruce L., and Arlan O. Benscoter. *Metallographer's guide: practice and procedures for irons and steels*. Asm International, 2001.

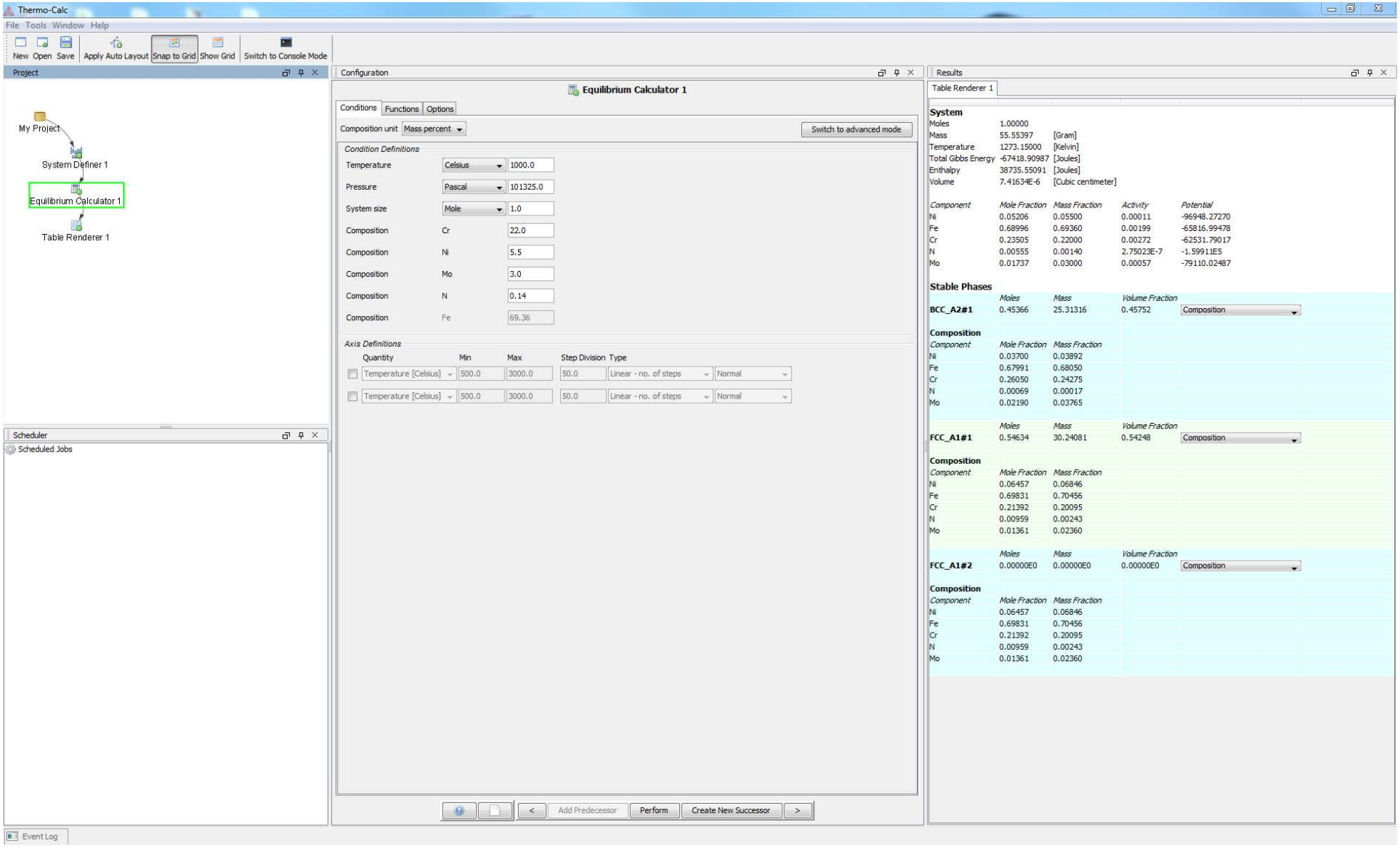
Single point equilibrium

Use the ”Quick Start” wizard
Calculate the equilibrium state for a steel under the following conditions:

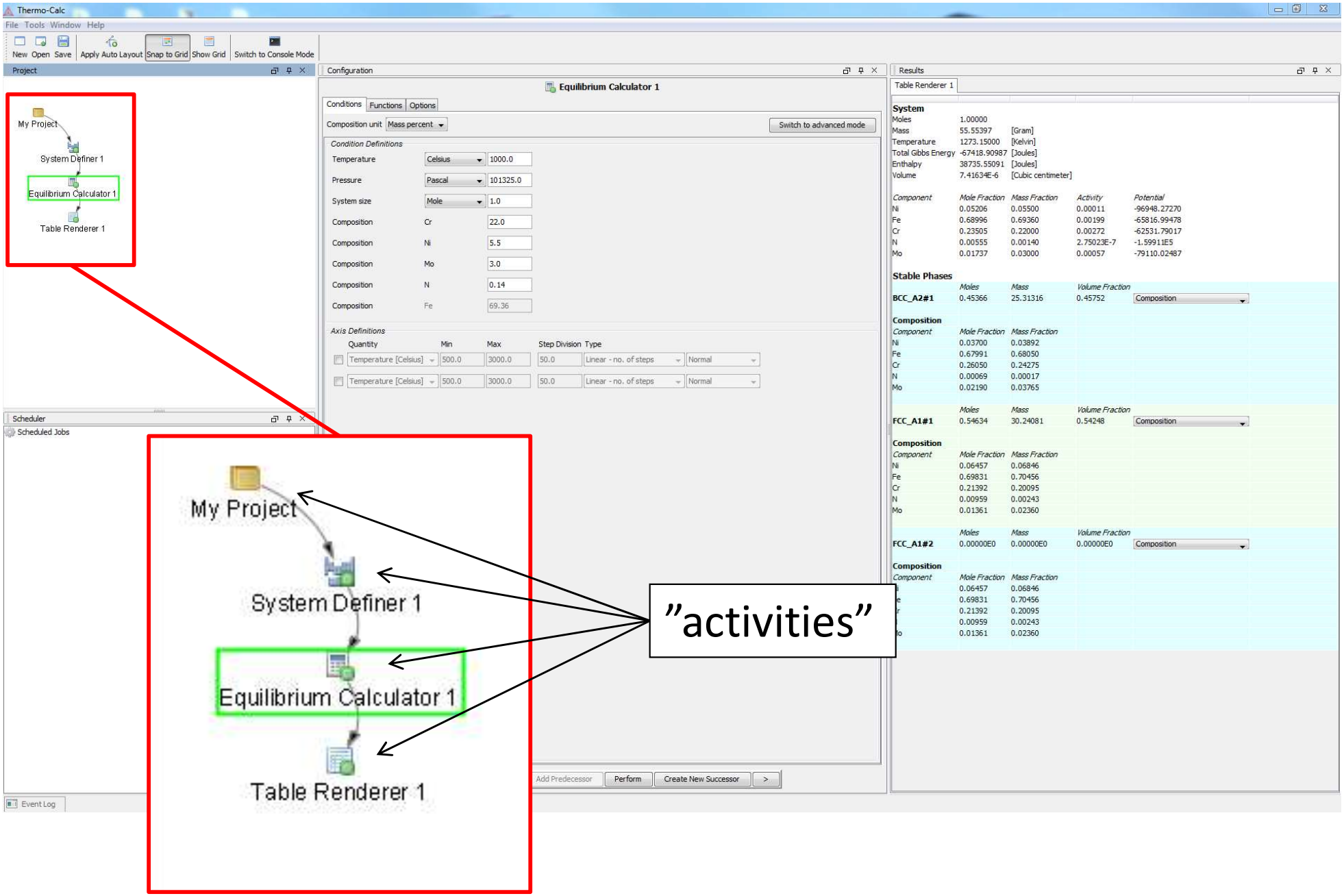
- Duplex 2205 – Fe - 22Cr – 5 Ni – 0.02C – 1.8Mn – 2.5Mo – 0.1N [mass-%] at 1050°C (typical solution annealing temp)
- A system size of 1 mole and atmospheric pressure is assumed



Single point equilibrium



Single point equilibrium



Single point equilibrium

Thermo-Calc Software

System

Moles	1.00000	
Mass	55.55397	[Gram]
Temperature	1273.15000	[Kelvin]
Total Gibbs Energy	-67418.90987	[Joules]
Enthalpy	38735.55091	[Joules]
Volume	7.41634E-6	[Cubic centimeter]

Component	*Mole Fraction*	*Mass Fraction*	*Activity*	*Potential*
Ni	0.05206	0.05500	0.00011	-96948.27270
Fe	0.68996	0.69360	0.00199	-65816.99478
Cr	0.23505	0.22000	0.00272	-62531.79017
N	0.00555	0.00140	2.75023E-7	-1.59911E5
Mo	0.01737	0.03000	0.00057	-79110.02487

Stable Phases

	Moles	*Mass*	*Volume Fraction*	
BCC_A2#1	0.45366	25.31316	0.45752	Composition

Composition

Component	*Mole Fraction*	*Mass Fraction*
Ni	0.03700	0.03892
Fe	0.67991	0.68050
Cr	0.26050	0.24275
N	0.00069	0.00017
Mo	0.02190	0.03765

	Moles	*Mass*	*Volume Fraction*	
FCC_A1#1	0.54634	30.24081	0.54248	Composition

Composition

Component	*Mole Fraction*	*Mass Fraction*
Ni	0.06457	0.06846
Fe	0.69831	0.70456
Cr	0.21392	0.20095
N	0.00959	0.00243
Mo	0.01361	0.02360

Thermo-Calc Software

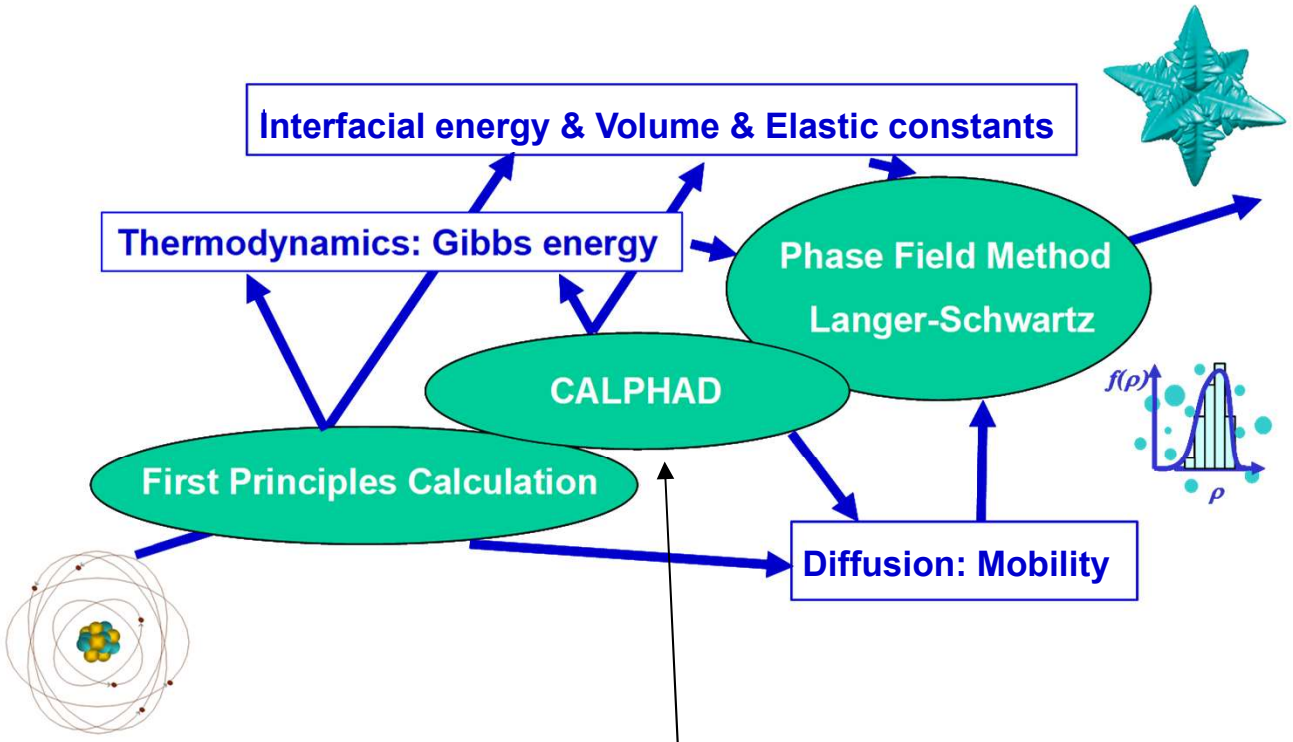
Introduction to Thermo-Calc and CALPHAD-based software tools

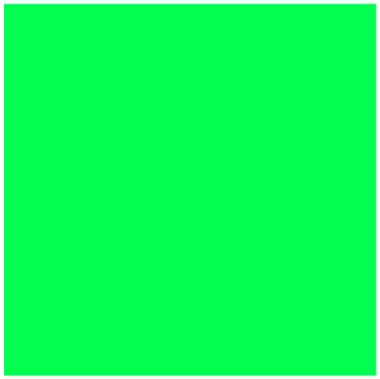
Our field of operation

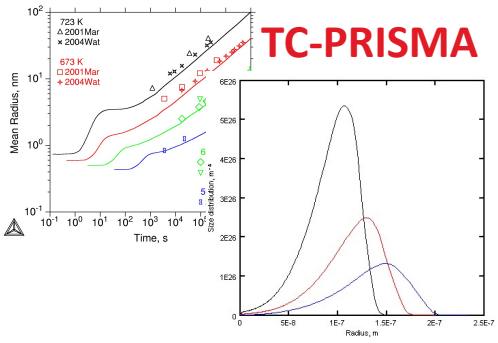
Thermo-Calc Software

Towards prediction of microstructure evolution and material properties

Bridging Atoms and Microstructure







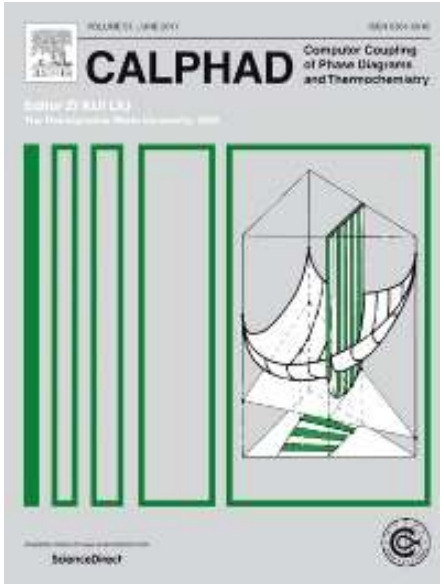
TC-PRISMA

The development of consistent databases where each phase is described separately using models based on physical principles and parameters assessed from experimental data is a key.

What is CALPHAD?

Thermo-Calc Software

CALculation of **PHA**se **D**iagrams

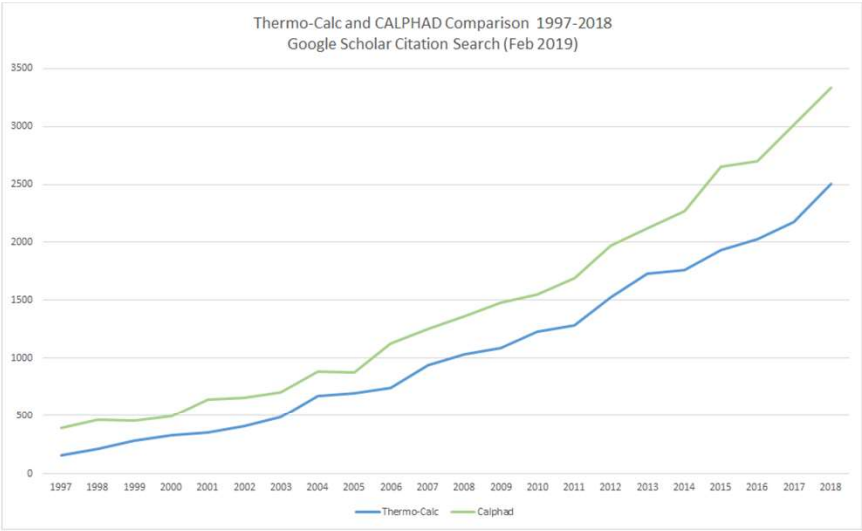


A phase based approach to modeling the underlying thermodynamics and phase equilibria of a system through a self consistent framework that allows extrapolation to multicomponent systems.

Captures the composition, temperature and pressure dependence.

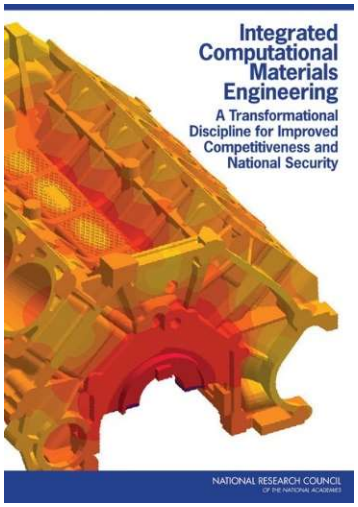
A journal published quarterly by Elsevier Ltd.

An international community, and conference held each year with 150-300 active participants from around the world.



ICME

Thermo-Calc Software



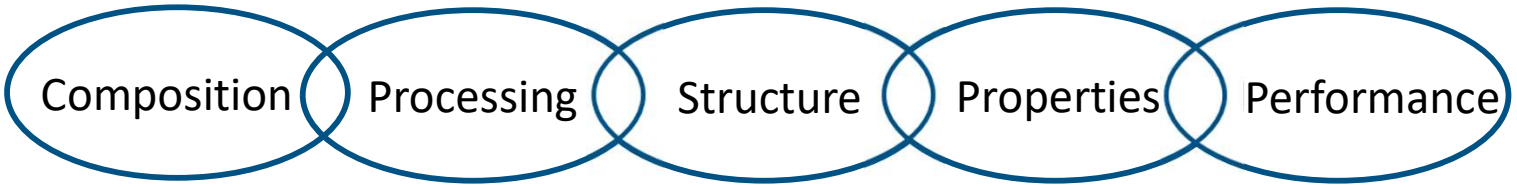
The National Academies Press, 2008

"Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security"

Moving beyond Materials Discovery…

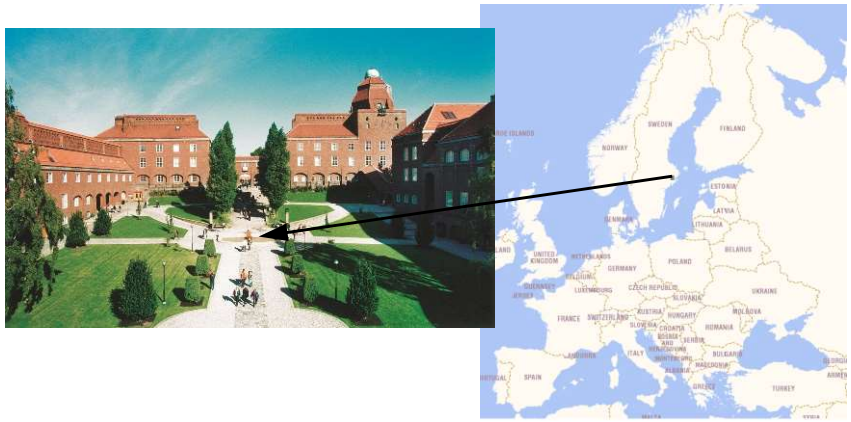
ICME: an approach to design products, the materials that comprise them, and their associated materials processing methods by linking materials models at multiple length scales.

Towards ICME:



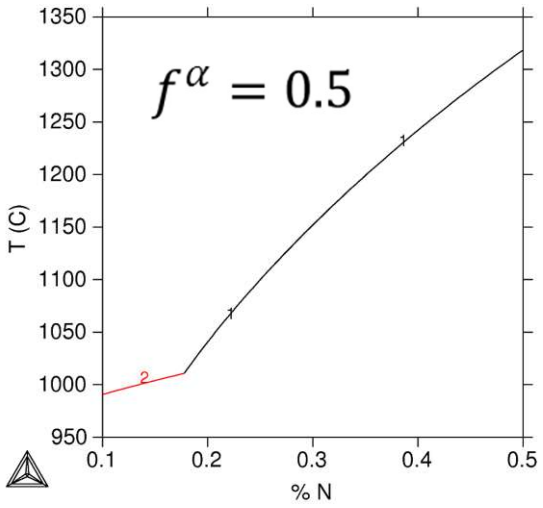
Thermo-Calc Software AB

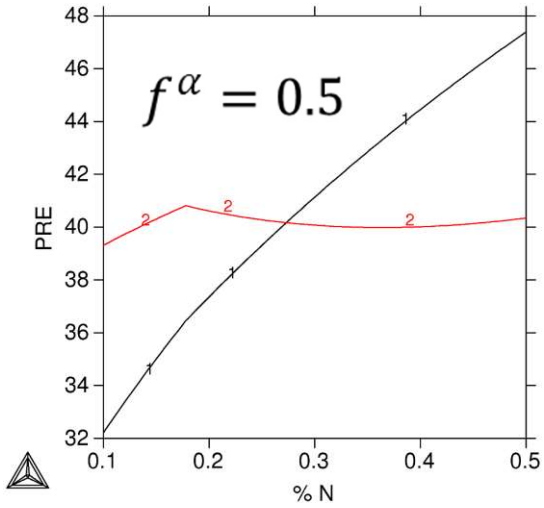
Thermo-Calc Software AB was founded in 1997 and originates in research that had been made at the Royal Institute of Technology, Stockholm, Sweden.



Sandvik and Nippon Steel are early adopters of these research tools in the mid 1980's.

A classic example from 1985 – SAF 2507





The company's mission is to further develop and extend these tools in order to meet today's and future needs.

Products and Services

- Software maintenance and support
  - Thermo-Calc (1984)
  - DICTRA (1992)
  - TC-PRISMA (2011)
  - Software Development Kits

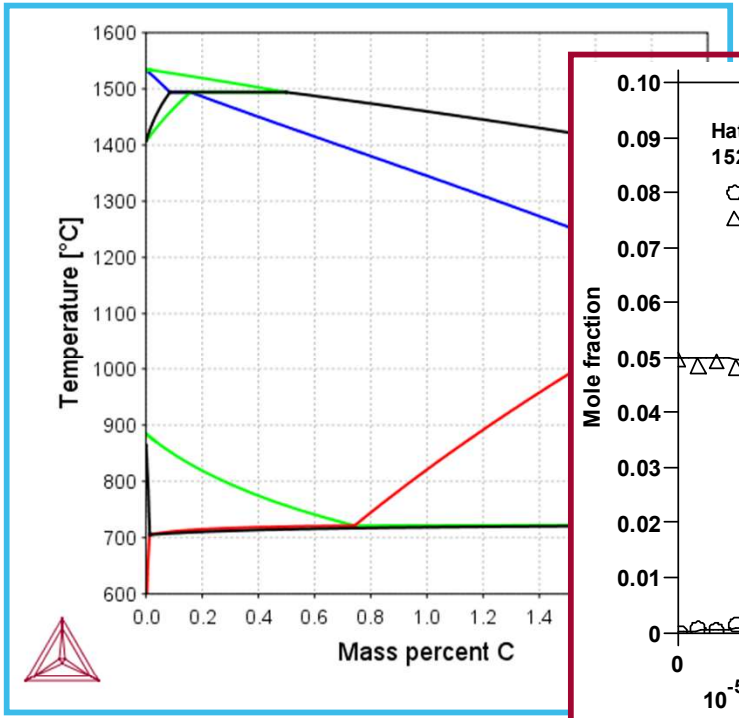
- Thermodynamic and Mobility databases

- Project work and consulting

- Training

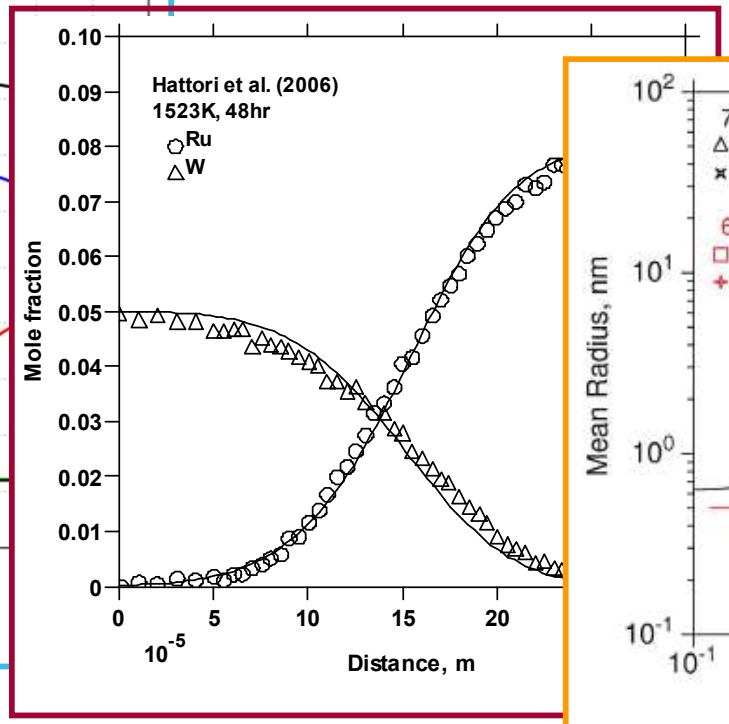
Developing Integrated Codes

Thermo-Calc Software



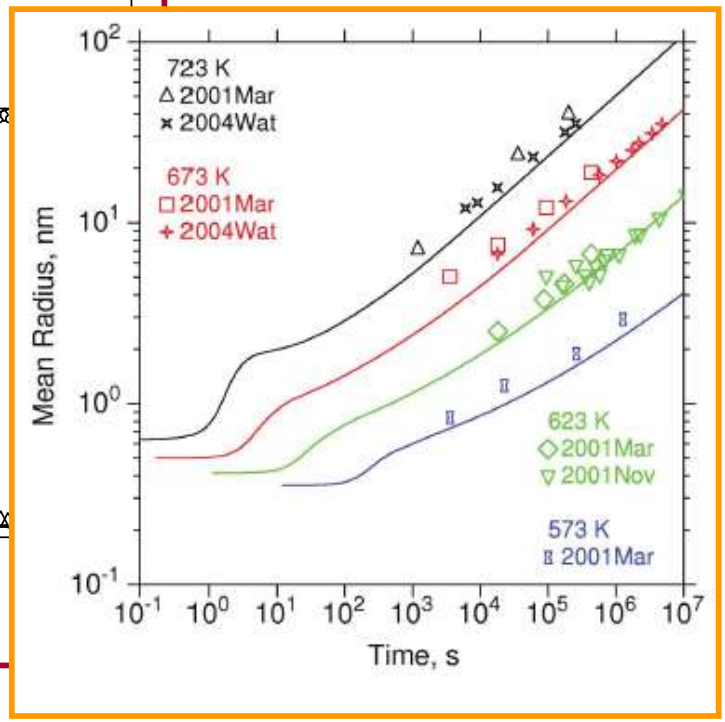
Gibbs energy
= Phase diagrams
(equilibrium & metastable also driving forces!)

Thermo-Calc software
for thermodynamic properties and phase equilibria



+ Mobility data
= Diffusion

Diffusion module
DICTRA



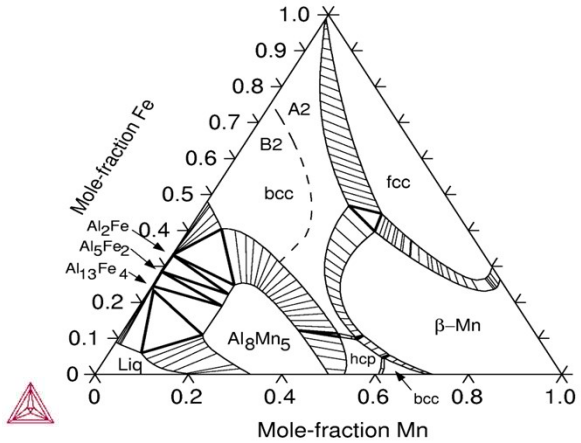
+ Interfacial energy
= Precipitation

Precipitation module
TC-PRISMA

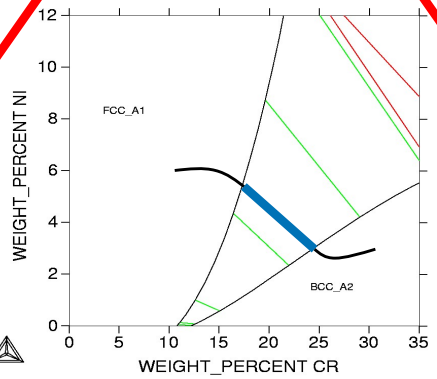
Developing Integrated Codes

Thermo-Calc Software

THERMO-CALC



Driving forces

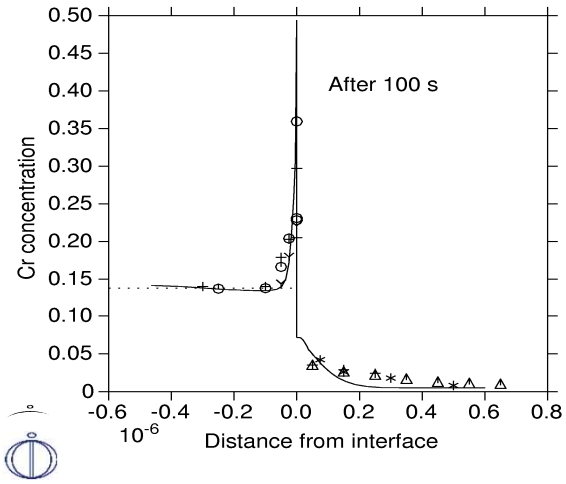


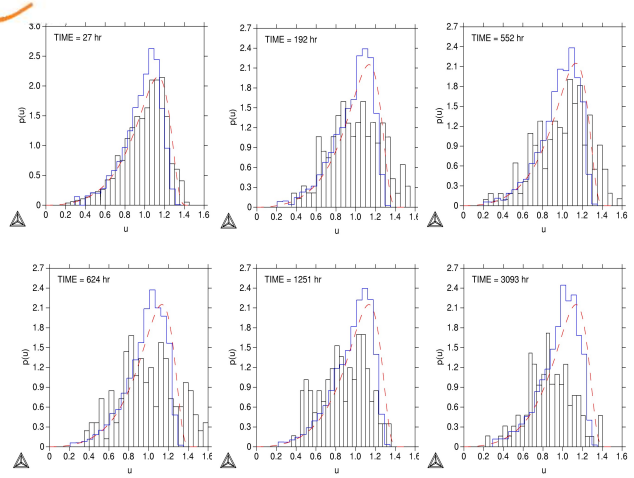
Interfacial energies

DICTRA

Diffusivities

TC-PRISMA





CALPHAD Background

Thermo-Calc Software

- CALPHAD based tools lie at the nexus of composition, temperature, property relationships.
- Phase based approach to modeling the composition/temperature dependence on Gibbs Energy
- Self-consistent framework allows for extrapolation into multi-component space, to explore what happens with real alloys, or to help guide development of new ones

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

Gibbs Free Energy

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

Ficks Laws of Diffusion

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

Classical Nucleation Theory

To use this approach, need to describe G, and D! (and σ and molar volume as well) – for each phase as a function of composition/temperature (CALPHAD Database)

Software + Databases

Thermo-Calc Software

Thermo-Calc

Minimization of the total Gibbs free energy under given conditions.

$$G = \sum_{\phi} N^{\phi} G_m^{\phi}\left(T, P, x_i^{\phi}\right)$$

$$\frac{\partial G}{\partial x_i^{\phi}} = 0$$

DICTRA

1-D diffusion simulation – Numerically solve diffusion equations

Solve Diffusion

$$\frac{\partial \mathbf{c}}{\partial t} = -\frac{\partial}{\partial z}(\mathbf{J}) \quad \text{where} \quad \mathbf{J} = -\mathbf{D}\frac{\partial \mathbf{c}}{\partial z}$$

TC-PRISMA

Mean field precipitation simulation – using LS (Langer-Schwartz) and KWN (Kampmann and Wagner Numerical) Approach

Continuity equation

$$\frac{\partial f(r,t)}{\partial t} = -\frac{\partial}{\partial r}\left[\upsilon(r) f(r,t)\right] + j(r,t)$$

$$C_0^{\alpha} = C^{\alpha} + \left(C^{\beta} - C^{\alpha}\right)\int_0^{\infty} \frac{4\pi}{3} f(r,t) r^3 dr$$

Mass balance

What can we calculate, predict, simulate?

Thermo-Calc Software

Thermo-Calc

- Stable/Metastable Equilibria
- Amount and composition of phases
- Transformation temps (liquidus, solidus, A1, A3, solvus etc)
- Density/Thermal expansion
- Solidification, segregation
- Enthalpy, heat capacity, latent heat etc.
- Phase diagrams
- (Thermo-)physical properties.

DICTRA

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

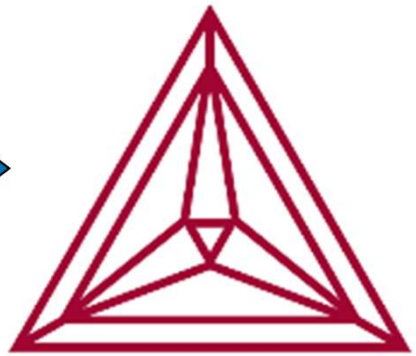
TC-PRISMA

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

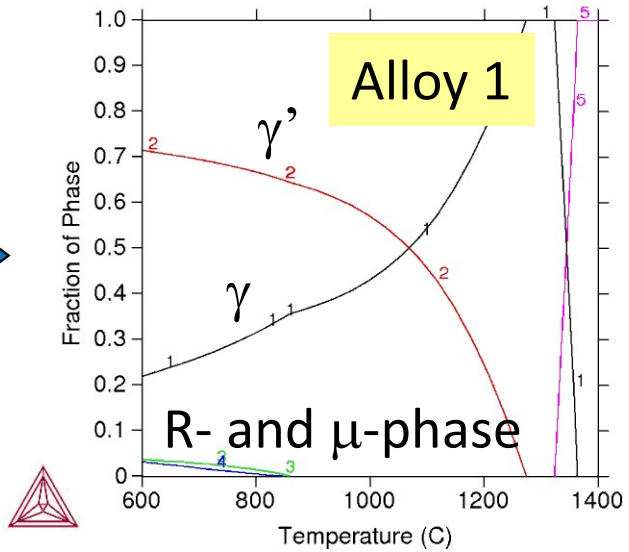
Thermo-Calc Software

Method

Thermodynamic Database



Thermo-Calc



Description of Gibbs free energy for the individual phases

$$G_m^{\phi}\left(T,P,x_i^{\phi}\right)$$

Minimization of the total Gibbs free energy under given conditions.

$$G=\sum_{\phi}N^{\phi}G_m^{\phi}\left(T,P,x_i^{\phi}\right)$$

$$\frac{\partial G}{\partial x_i^{\phi}}=0$$

Result

Thermo-Calc Software

Example of functionality

- Calculating stable and meta-stable heterogeneous phase equilibrium
- Amount and composition of phases
- Transformation temperatures, e.g. liquidus and solidus temperature
- Predicting driving forces for phase transformations
- Phase diagrams (binary, ternary, isothermal, isoplethal, etc.)
- Molar volume, density and thermal expansion
- Physical properties, e.g. viscosity, thermal conductivity
- Scheil-Gulliver (non-equilibrium) solidification simulations
- Thermochemical data such as;
  - enthalpies
  - heat capacity,
  - activities, etc.
- Thermodynamic properties of chemical reactions
- And much more….

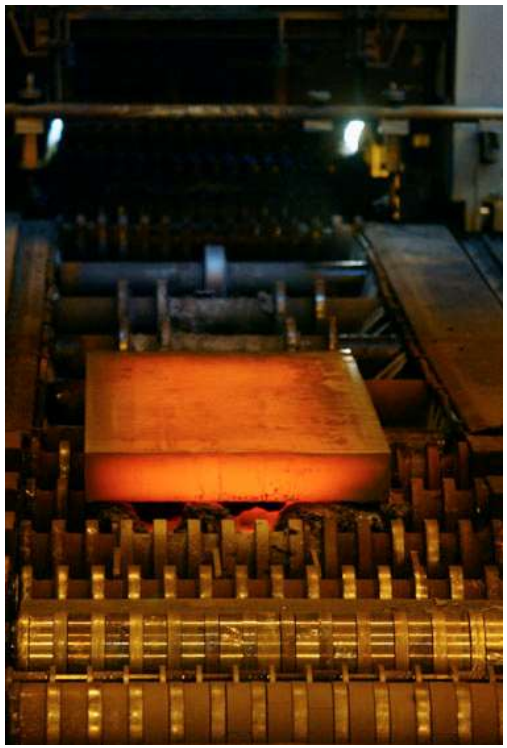


Photo: Stig-Göran Nilsson (2002)

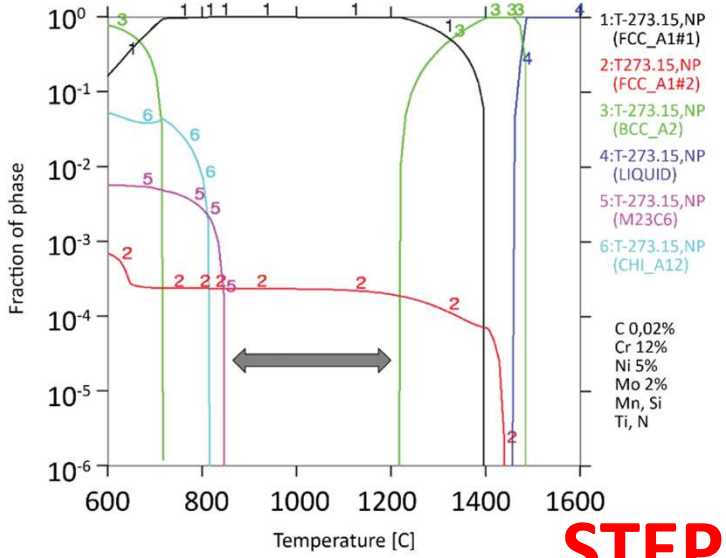
- Design and optimization of alloys
- Design and optimization of processes
- Analyze and gain understanding of problems
- …..

Fundamental types of calculations

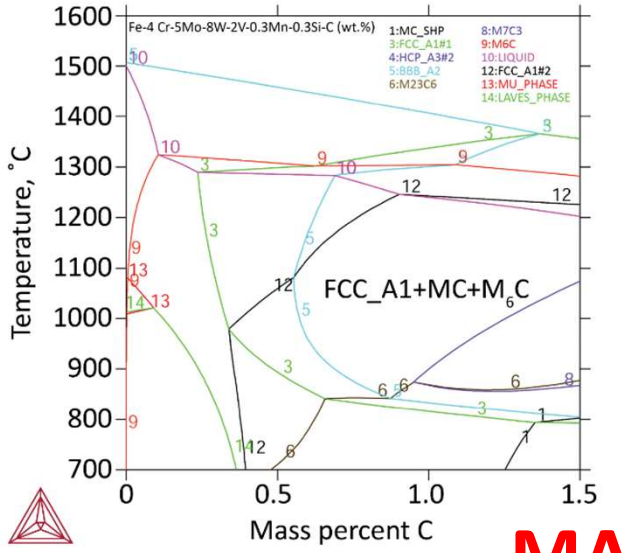
Thermo-Calc Software

```
Output from POLY-3
Tue Aug 08 2006 11:41:39

Database: TCFE3

Conditions:
T=1000, P=1E5, N=1, W(C)=2E-2, W(CR)=0.1, W(MN)=3E-2, W(NI)=1E-2
DEGREES OF FREEDOM 0

Temperature 1000K (727C, 1340F),  Pressure 1.000000E+05
Number of moles of components 1.00000E+00,  Mass 5.16905E+01
Total Gibbs energy -4.42393E+04,  Enthalpy 2.56582E+04,  Volume 5.22429E-06

Component        Moles          W-Fraction     Activity       Potential      Ref.State

C                8.6072E-02     2.0000E-02     8.9724E-02     -2.0046E+04    SER
CR               9.9412E-02     1.0000E-01     4.4290E-04     -6.4206E+04    SER
FE               7.7748E-01     8.4000E-01     6.0347E-03     -4.2489E+04    SER
MN               2.8227E-02     3.0000E-02     4.6517E-05     -8.2943E+04    SER
NI               8.8074E-03     1.0000E-02     3.3158E-05     -8.5758E+04    SER


FCC_A1#1         STATUS  ENTERED              Driving force  0.0000E+00
Number of moles 7.5868E-01, Mass 4.1735E+01
Mass fractions:
FE  9.44835E-01   CR  1.41596E-02   C   3.93605E-03
MN  2.47653E-02   NI  1.23038E-02

FCC_A1#2         STATUS  ENTERED              Driving force  0.0000E+00
Number of moles 0.0000E+00, Mass 0.0000E+00
Mass fractions:
FE  9.44835E-01   CR  1.41596E-02   C   3.93605E-03
MN  2.47653E-02   NI  1.23038E-02

M7C3#1   STATUS  ENTERED                Driving force  0.0000E+00
Number of moles 2.4132E-01, Mass 9.9559E+00
Mass fractions:
CR  4.59839E-01   C   8.73393E-02   NI  4.76[illegible]E-02
FE  4.00536E-01   MN  5.19435E-02
```

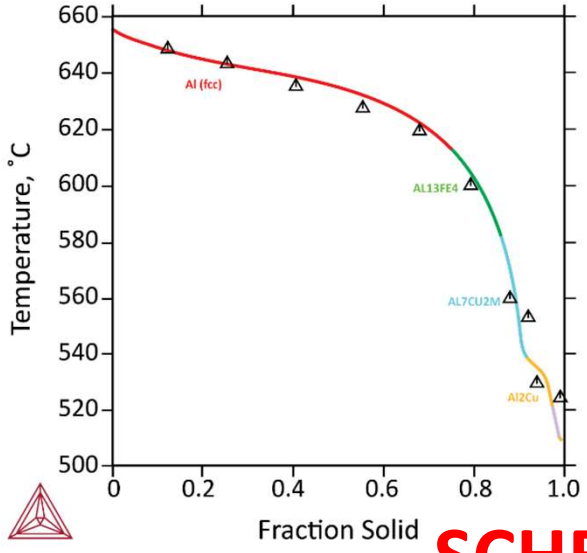
Single Point Equil.



STEP



MAP



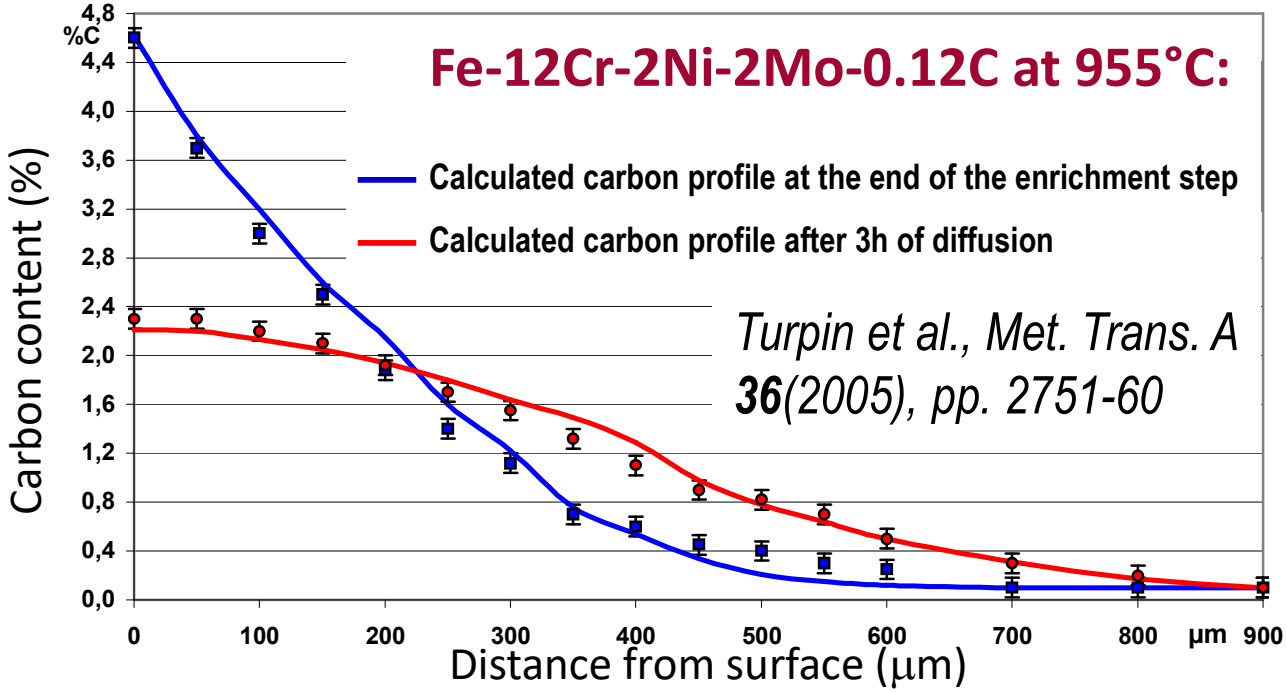
SCHEIL

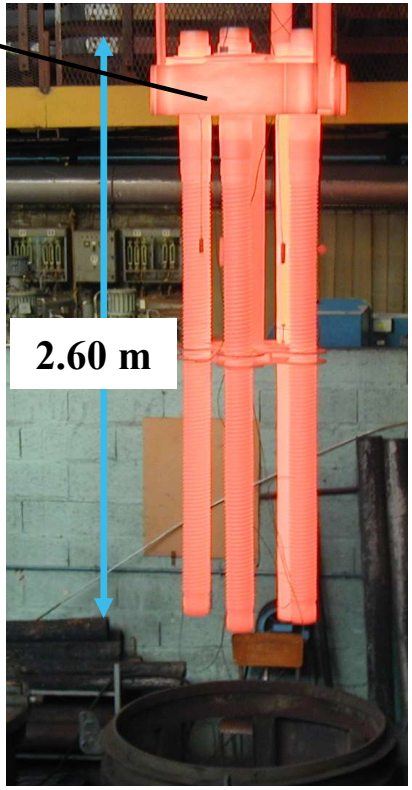
Diffusion module (DICTRA)

- Carburizing and decarburization
- Microsegregation during solidification
- Homogenisation treatment
- Precipitate growth and dissolution
- Precipitate coarsening
- Interdiffusion in coating/substrate systems
- TLP bonding of alloys and much more…

Ball screw for the Airbus A380 aircraft: a martensitic as carburized stainless steel

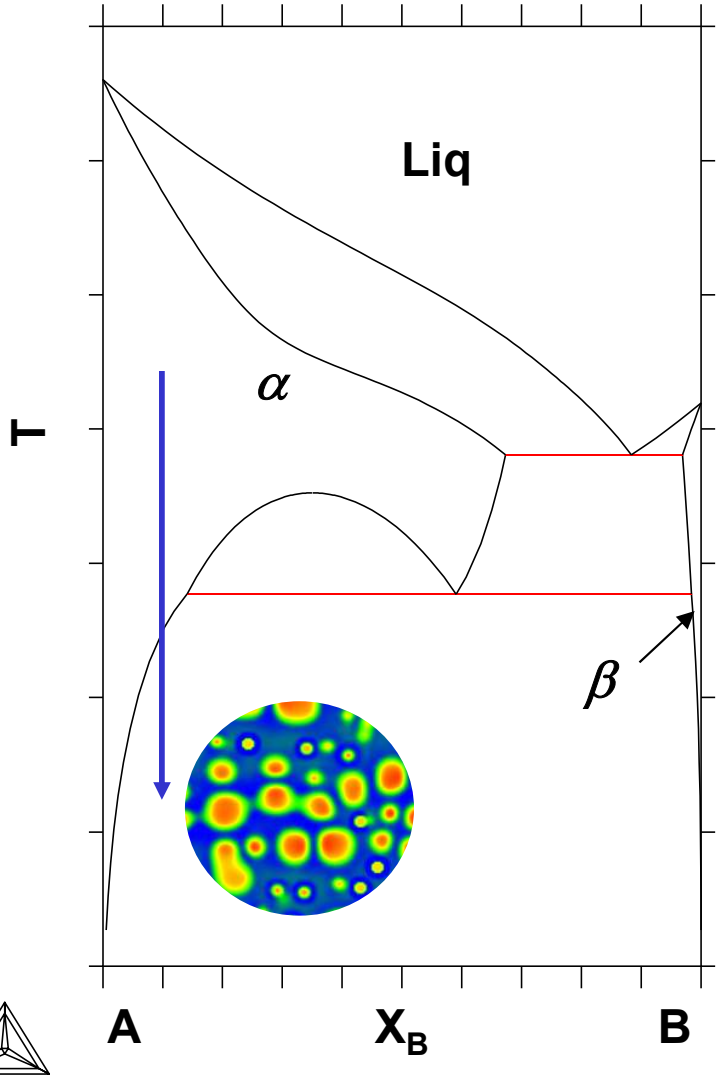
Example: Simulation of carbon evolution in high alloyed steels by Aubert & Duval, France.





Precipitation module (TC-PRISMA)

- Simulate concurrent nucleation, growth and coarsening of second phases in multicomponent systems.
- Integrated directly with Thermo-Calc and the Diffusion module (DICTRA).



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

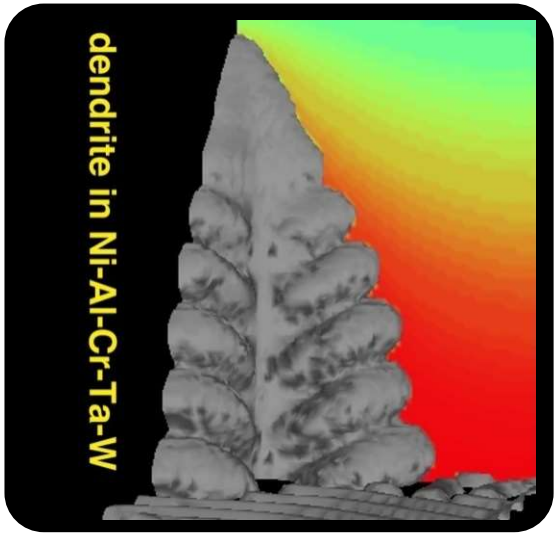
Software Development Kits (SDKs)

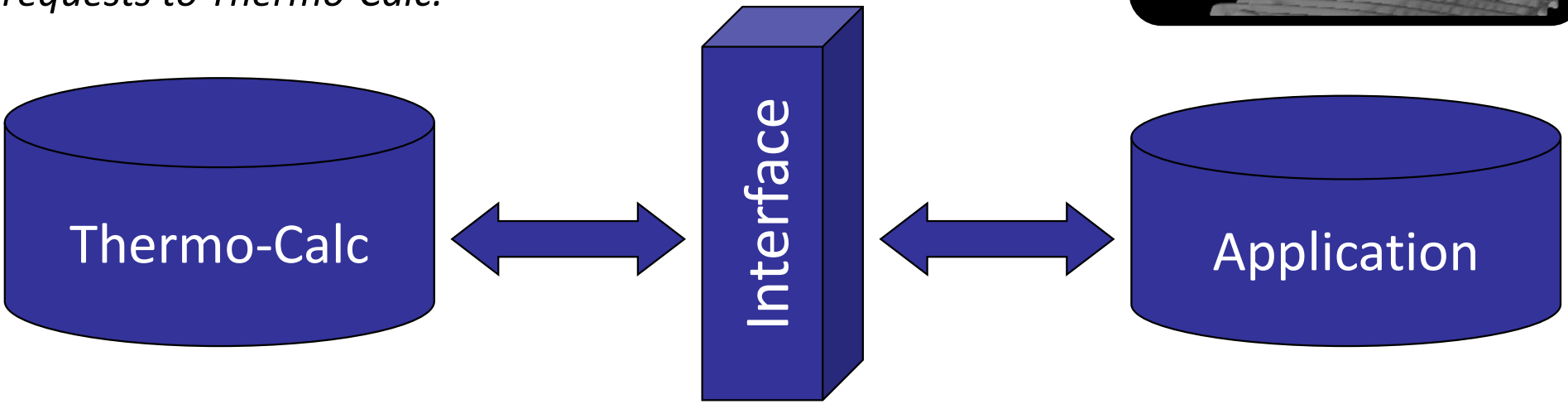
TC-Python / TQ-interface /

TC Toolbox for Matlab™

A prescribed set of subroutines, functions or classes by which a programmer writing an application program can make requests to Thermo-Calc.

Microstructure modelling





The trend is towards more and more advanced applications and in particular integration of thermodynamic calculation result for modelling of microstructure evolution and property prediction, aiming at designing products including the materials they consist of and their associated processing.

Databases

A database in our understanding means *a collection of polynomials describing some property for the individual phases of a system, as a function of temperature, (pressure) and composition.*

- ❑ Thermodynamic data ⇒ All our software tools
  - Gibbs free energy, i.e. $G_m^{\phi} = f\left(T, P, x_i^{\phi}\right)$

- ❑ Kinetic data ⇒ DICTRA, TC-PRISMA, (TC-API's)
  - Atomic mobility

- ❑ Property data
  - Molar volume ⇒ TC, TC-PRISMA, (TC-API's)
  - *Interfacial energies* ⇒ TC-PRISMA

Available Thermodynamic Databases

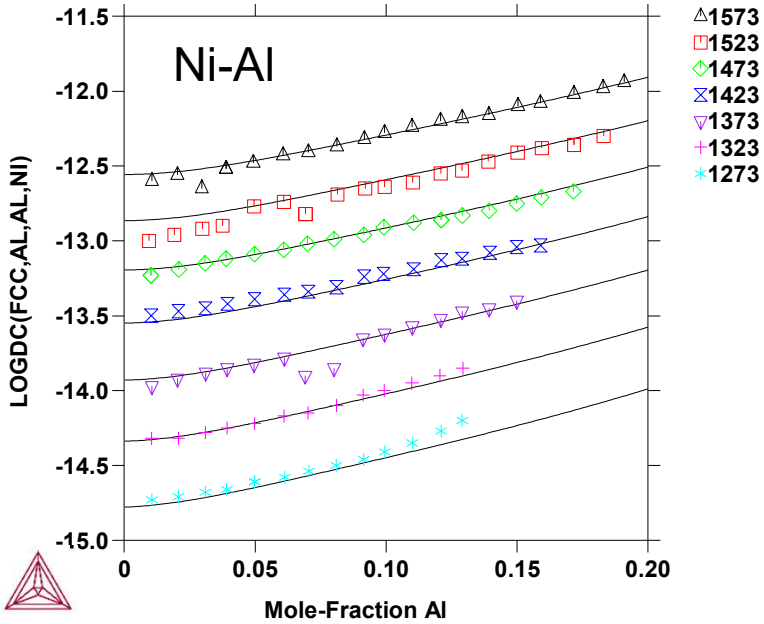
Thermo-Calc Software

A wide range of thermodynamic databases are available for:

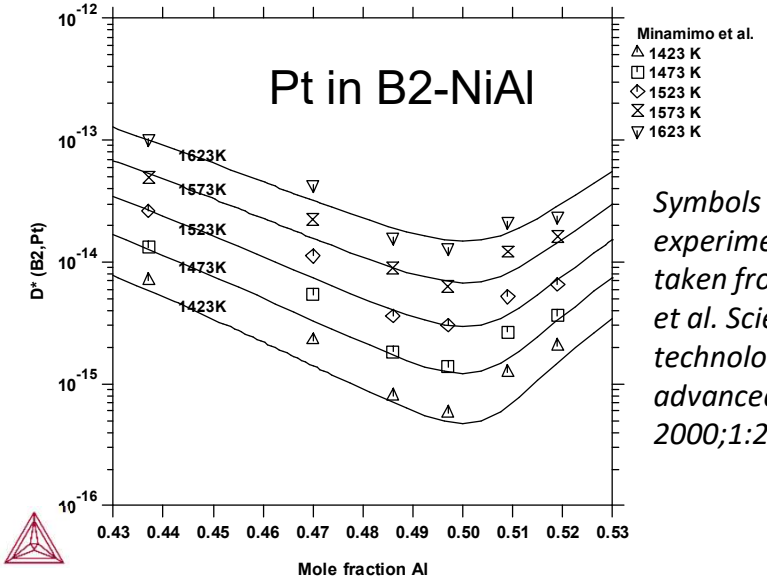
- Steels and Fe-alloys
- Nickel-base superalloys
- Al-/Ti-/TiAl-/Mg-/Cu-/Zr-alloys
- High Entropy alloys (HEA)
- Noble metal alloys, Solder alloys
- Electronic materials, magnetic materials, ultra-pure Si-alloys
- Gases, pure inorganic/organic substances and general alloys
- Slag, metallic liquids and molten salts
- Ceramic systems, hard materials, ultra-high temperature alloys
- Materials processing, process metallurgical and environmental aspects
- Aqueous solutions, materials corrosion and hydrometallurgical systems
- Minerals and geochemical/environmental processes
- Nuclear materials and nuclear fuel/waste processing

Available Kinetic Databases

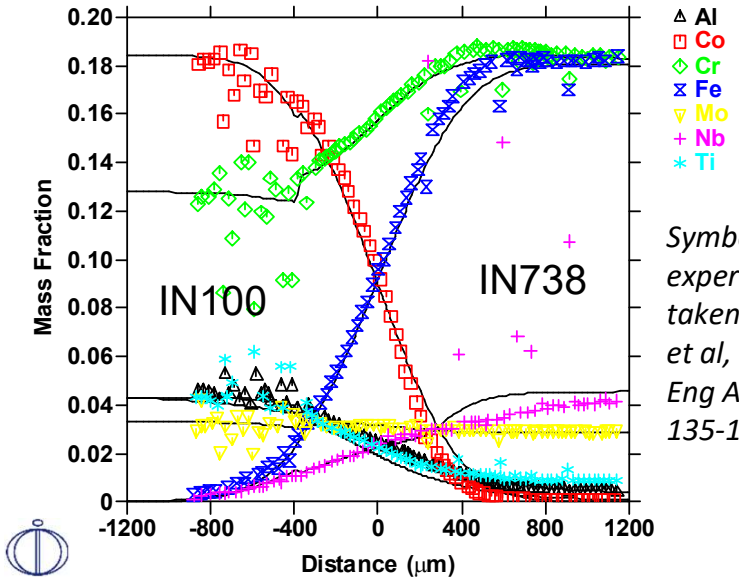
- ❑ Steels and Fe-alloys
- ❑ Nickel-base superalloys
- ❑ Aluminium alloys
- ❑ Noble metal alloys
- ❑ High Entropy alloys
- ❑ Ti alloys
- ❑ Cu alloys
- ❑ Mg alloys
- ❑ Solder alloys
- ❑ Si



*Symbols are experimental data taken from Yamamoto et al, Trans. Jpn. Inst. Met. **21**(1980), p. 601.*



Symbols are experimental data taken from Minamino et al. Science and technology of advanced materials 2000;1:237-249.



*Symbols are experimental data taken from Campbell et al, Materials Sci & Eng A **407**(2005), pp. 135-146.*

Customers

- Industry
  - Steel and metal producing companies
  - Manufacturing companies
    - Automotive
    - Electronics and semi-conductors
    - Aerospace & defense
    - Industrial equipment
    - Naval, maritime
    - Consumer goods
  - Energy & environment
  - Consulting services
- Governmental labs
- Academia *(material science, mech. engineering, metallurgy….)*



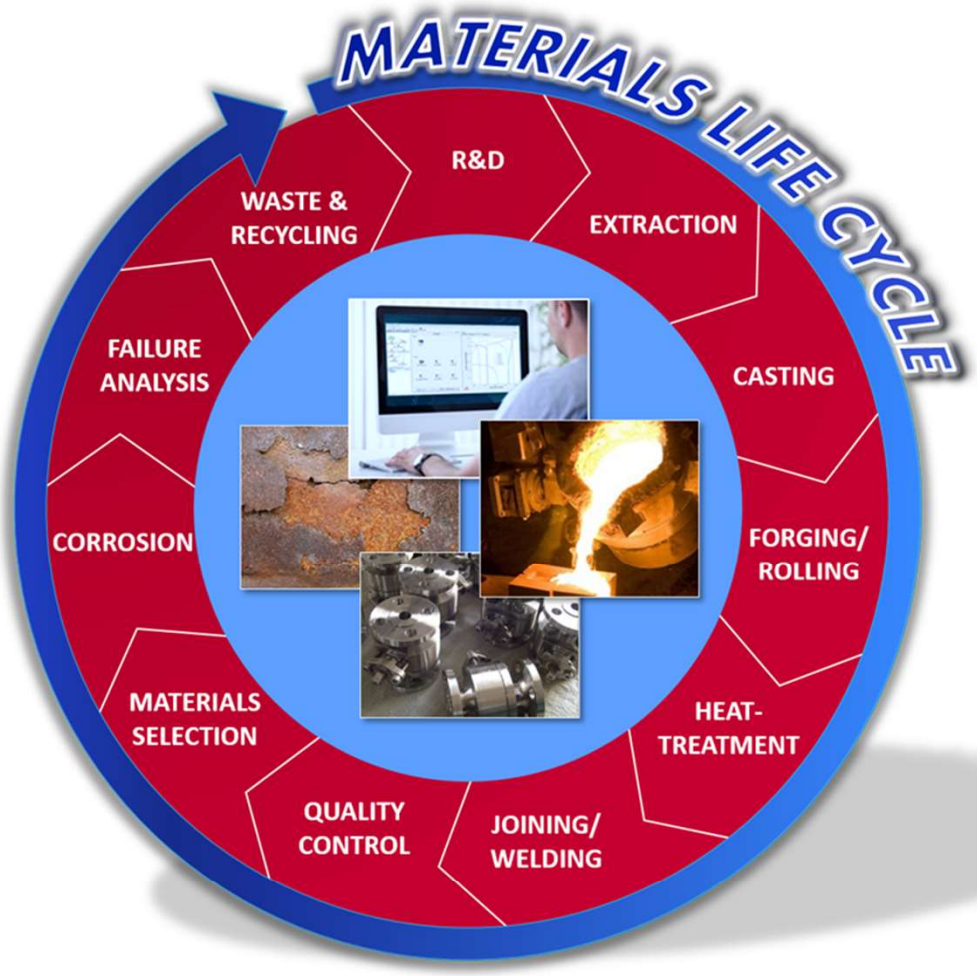







Examples with application to the materials life cycle

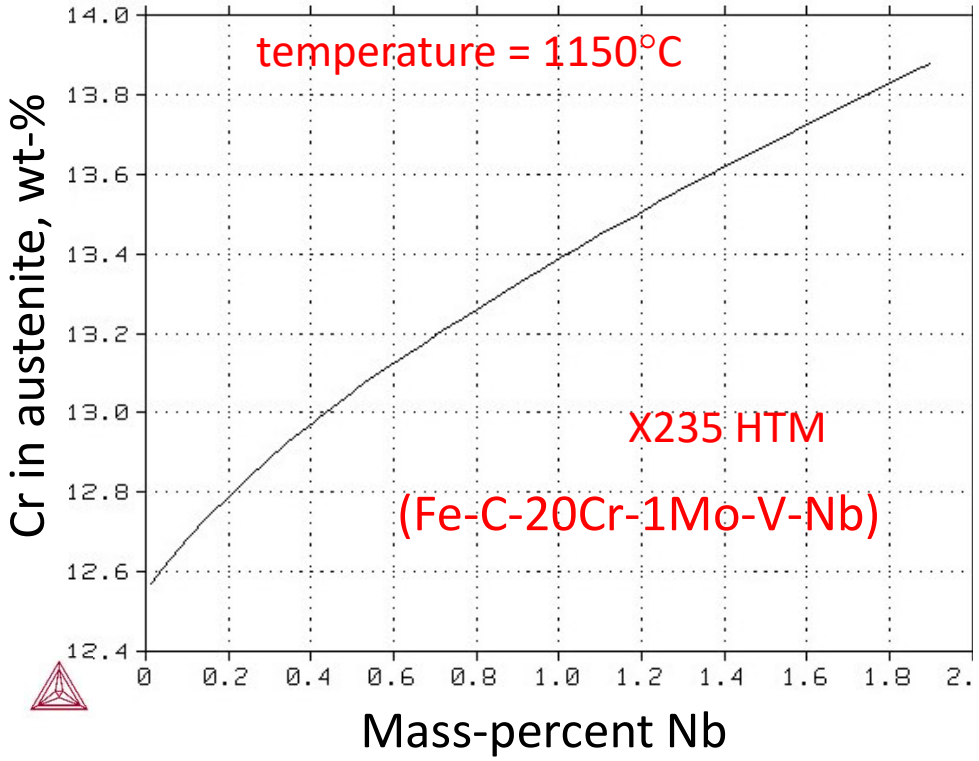
To provide computational tools in the field of materials engineering that allow for faster, cheaper and more sustainable innovation, development and production of both materials and components.

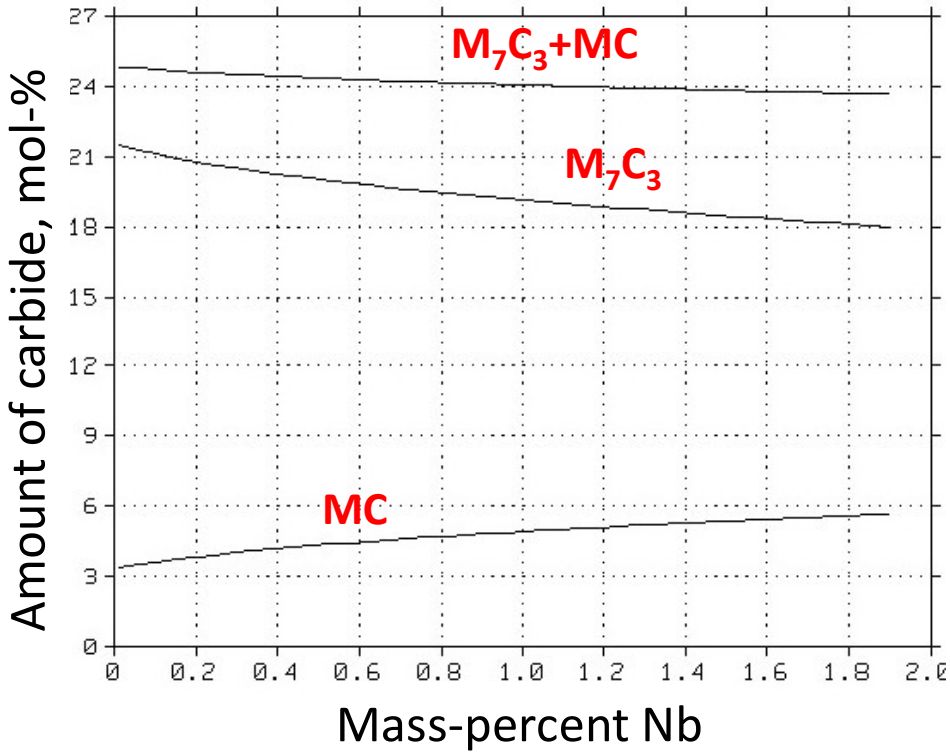


Thermo-Calc Software

Ascertaining the Influence of Alloying Elements

Example: Influence on Chromium solubility when replacing V with Nb





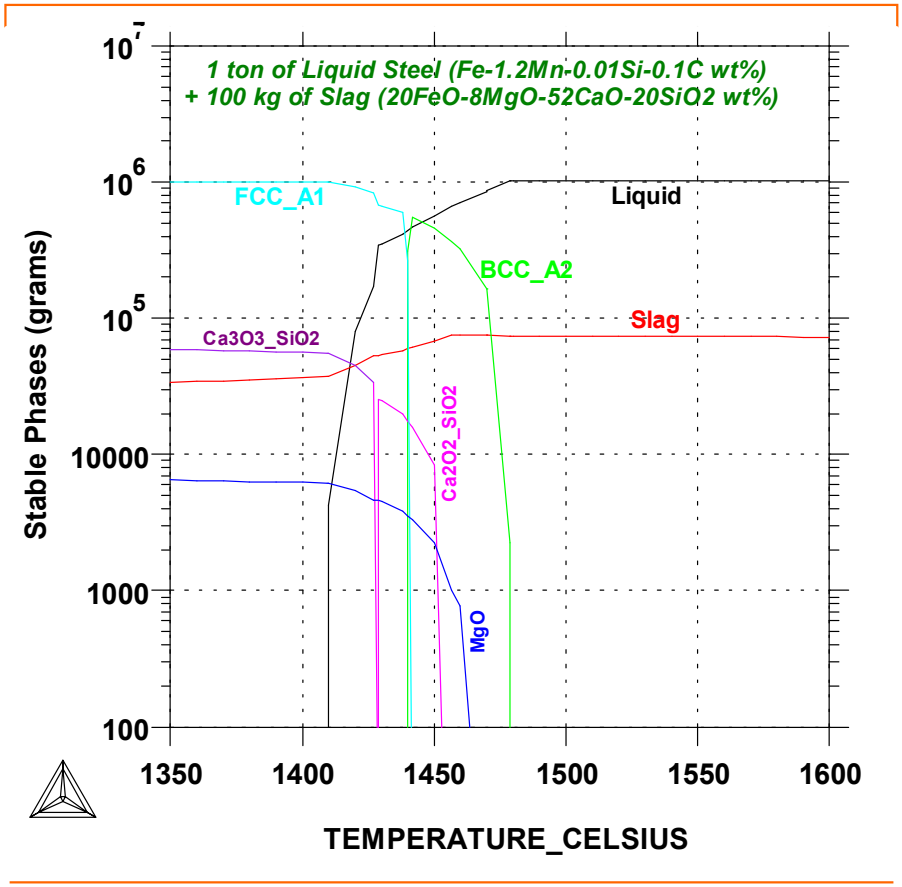
V + Nb = constant = 5.27 at. %

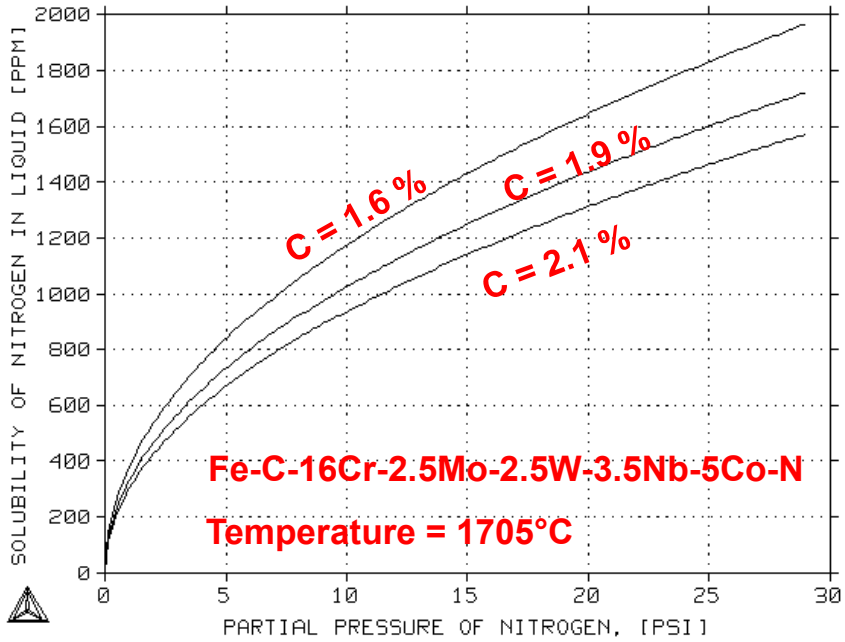
Metallurgical Extraction

Thermo-Calc Software

Several examples, e.g.

- ❑ Controlling and designing slag systems
- ❑ Interaction between slag and liquid metal
- ❑ Influence of an external pressure
- ❑ The Process Metallurgy Module





Casting

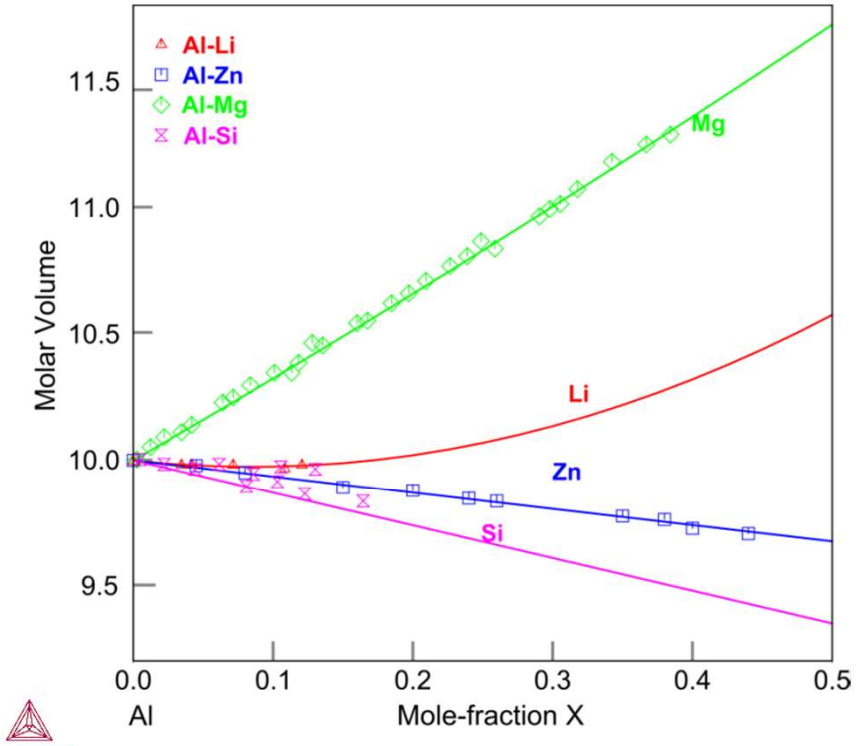
Thermo-Calc can be used to generate data to input into casting codes

- Solidus/liquidus temperatures
- Fraction solid curve
- Specific heat
- Thermal expansion coefficients
- Density / Molar volume
- Viscosity of Liquid phase

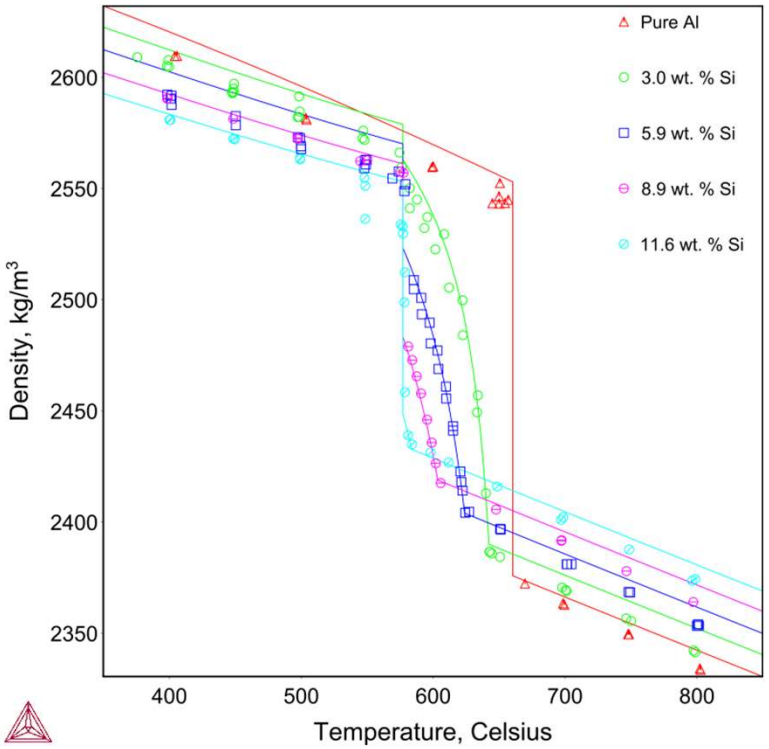
These quantities can of course also be used inside Thermo-Calc itself, see next page.

Thermo-Calc Software

Example: Predicting cast shrinkage for Al alloys



Calculated molar volumes of the Al-X (X=Li, Mg, Si, Zn) fcc_A1 phase



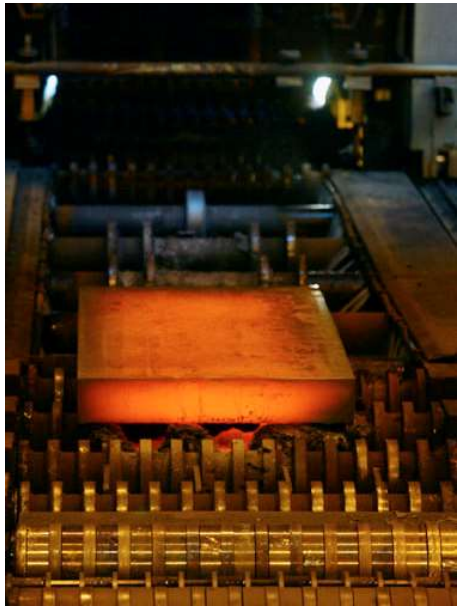
The effect of Si content on the densities of Al-Si alloys

Heat Treatment

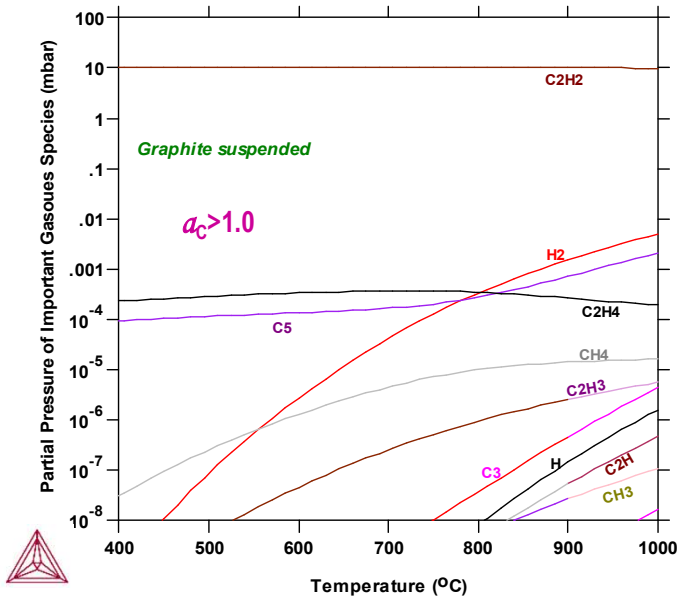
Thermo-Calc Software

Applications to a wide range of heat treatment related simulations, for instance:

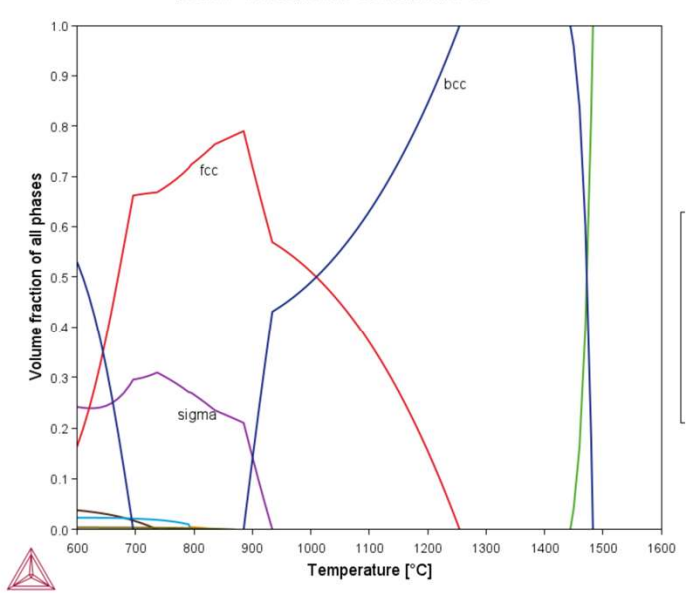
- Equilibrium between alloy and gas phase as a function of temperature and composition
- Predict formation of phases / volume-fractions etc.
- Gas phase reactions, gas speciation
- Oxide scale formation



Decomposition of Acetylene at 10 mbar



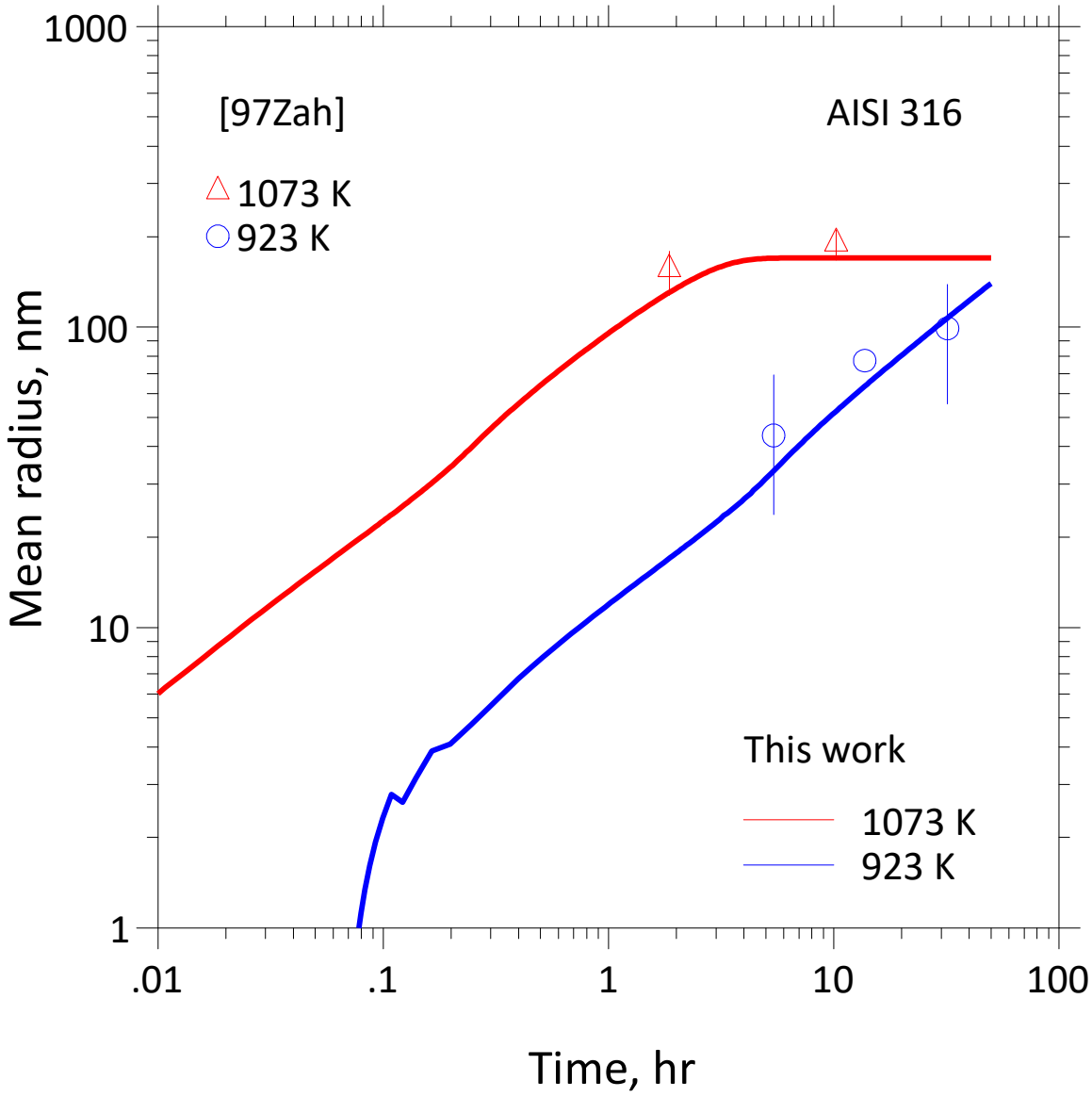
Phases in stainless steel



Heat Treatment

Thermo-Calc Software

TC-PRISMA simulation of precipitation kinetics of M23C6 in AISI 316



Input data for simulation:

- ❑ Thermodynamic & kinetic data
- ❑ Composition
  - C 0.08%
  - Cr 18%
  - Ni 12%
  - Mo 2%
  - Mn 1.5%
- ❑ Time & temperature
- ❑ Nucleation at grain boundaries

650 °C

γ-grain size = 100 μm

σ = 0.3 J/m^2

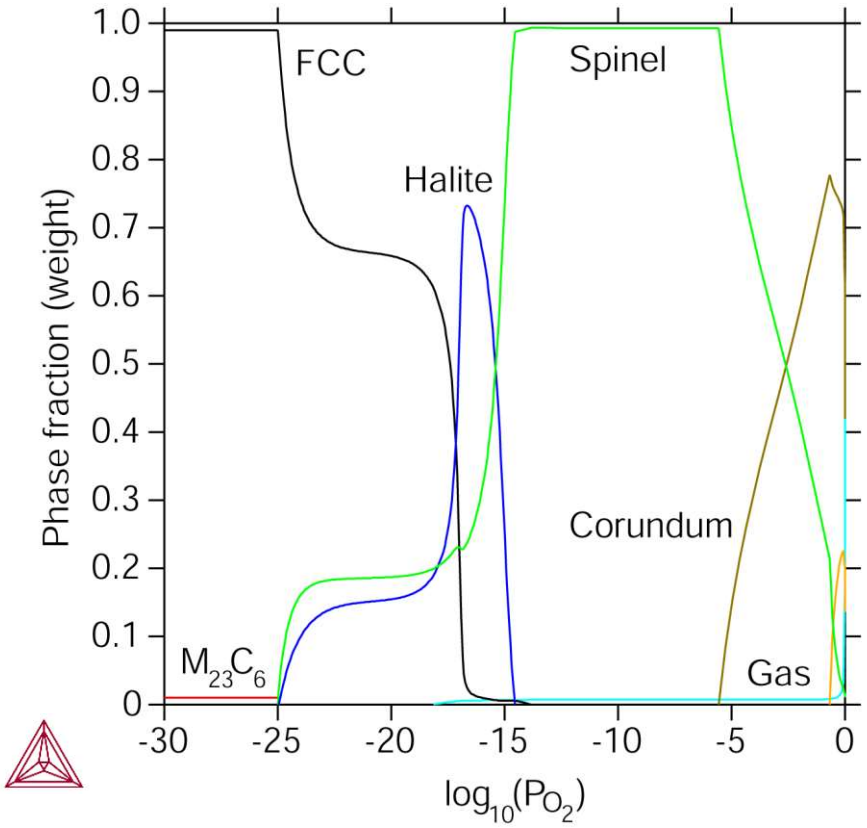
800 °C

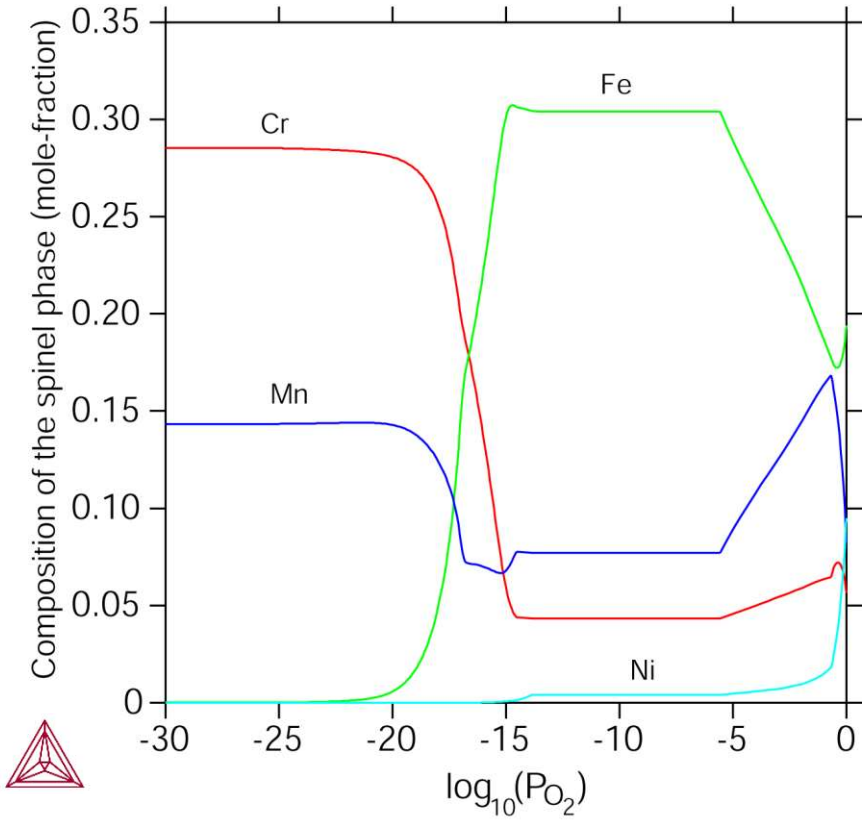
γ-grain size = 1000 μm

σ = 0.2 J/m^2

Heat Treatment

Oxide scale formation at 900 ºC on a steel with 17.8% Mn, 9.5% Cr, 1.0% Ni and 0.27% C





Below the outer scale (rich in corundum) an Fe-Mn rich spinel is formed and next to the substrate a layer with halite and a Cr-Mn rich spinel, which is verified experimentally in the work by Douglas et al [1].

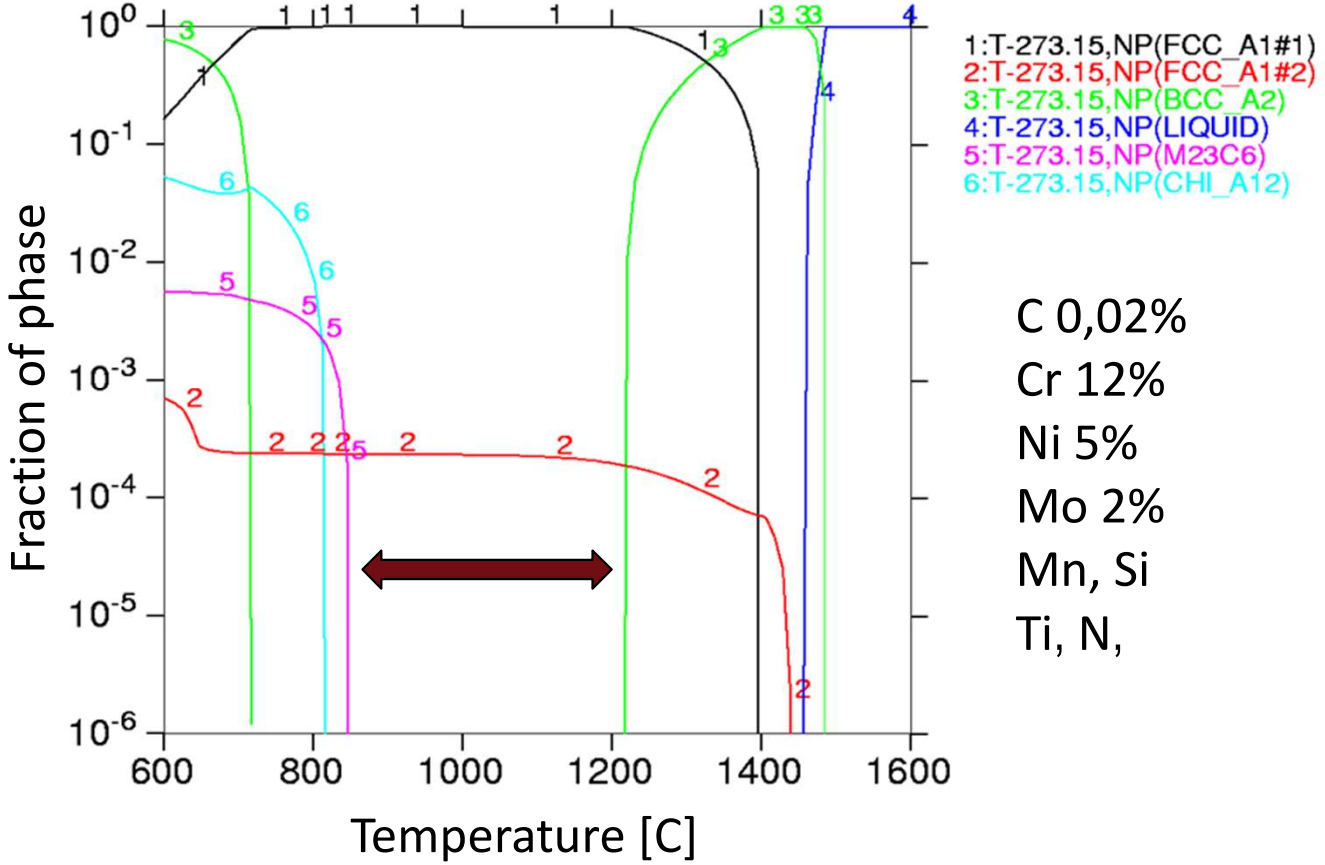
[1] D. L. Douglas, F. Gesmundo and C. De Asmundis, Oxidation of Metals, Vol. 25, 1986, pp. 235-268.

Forging/Rolling

Examples of use related to forging/rolling of metals e.g.

Selecting optimum temperature for operation

Safe forging of super-martensitic stainless in γ-field



C 0,02%
Cr 12%
Ni 5%
Mo 2%
Mn, Si
Ti, N,

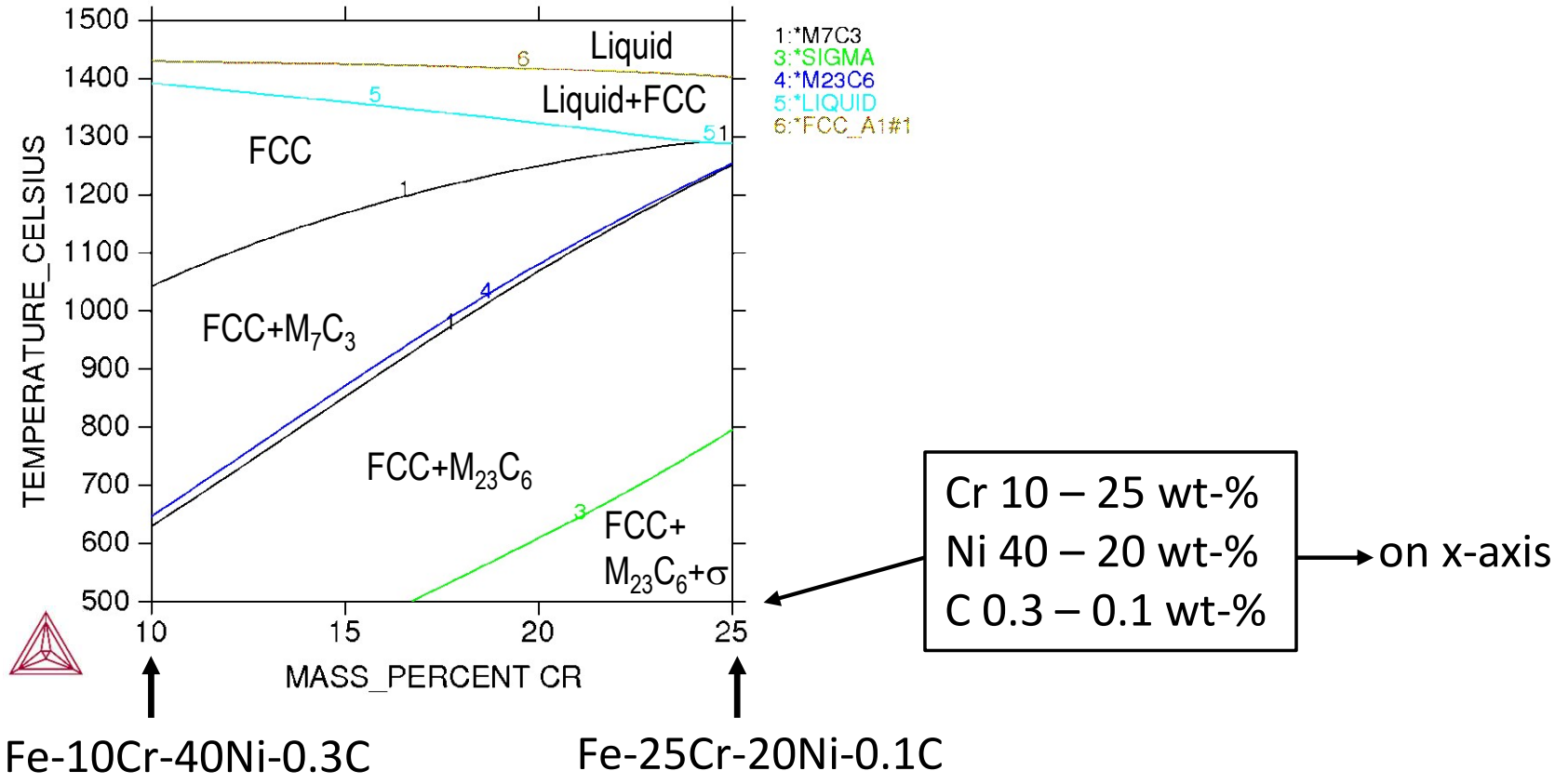
Courtesy André Costa e Silva

Joining/Welding

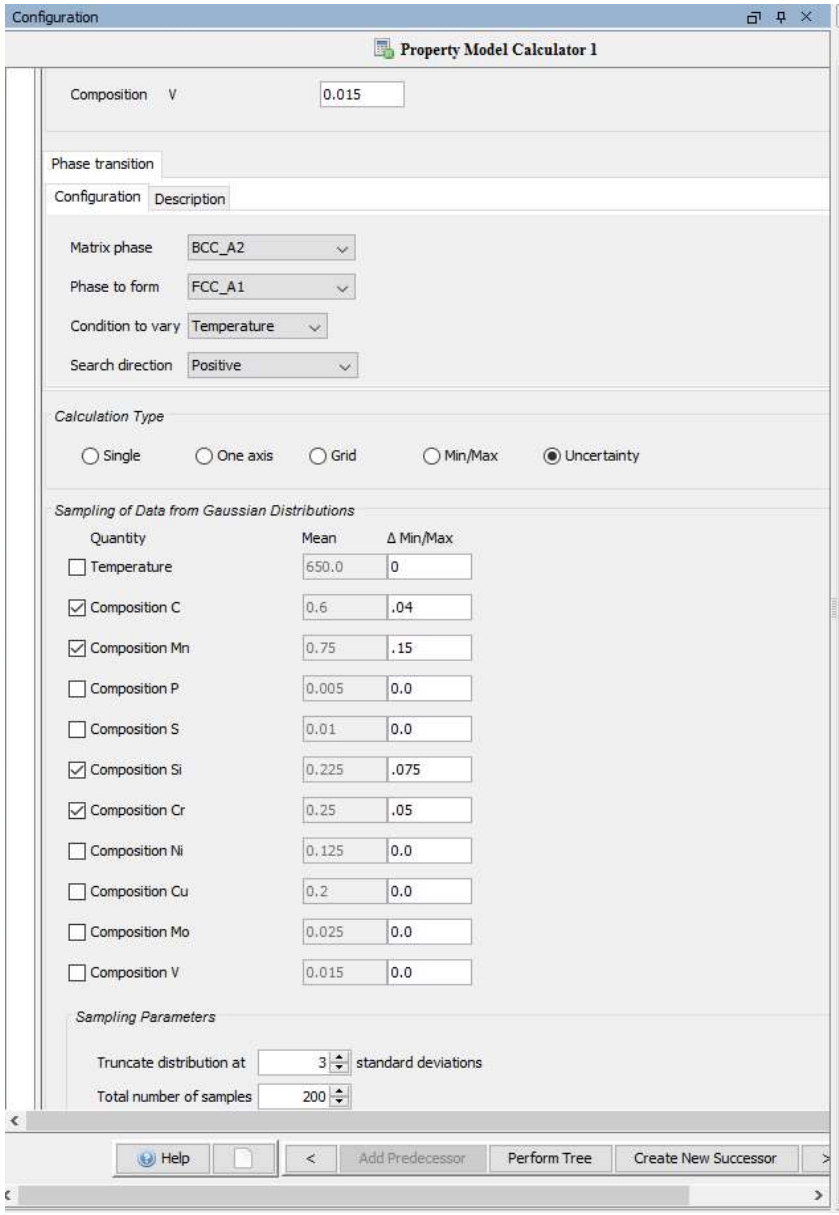
Thermo-Calc Software

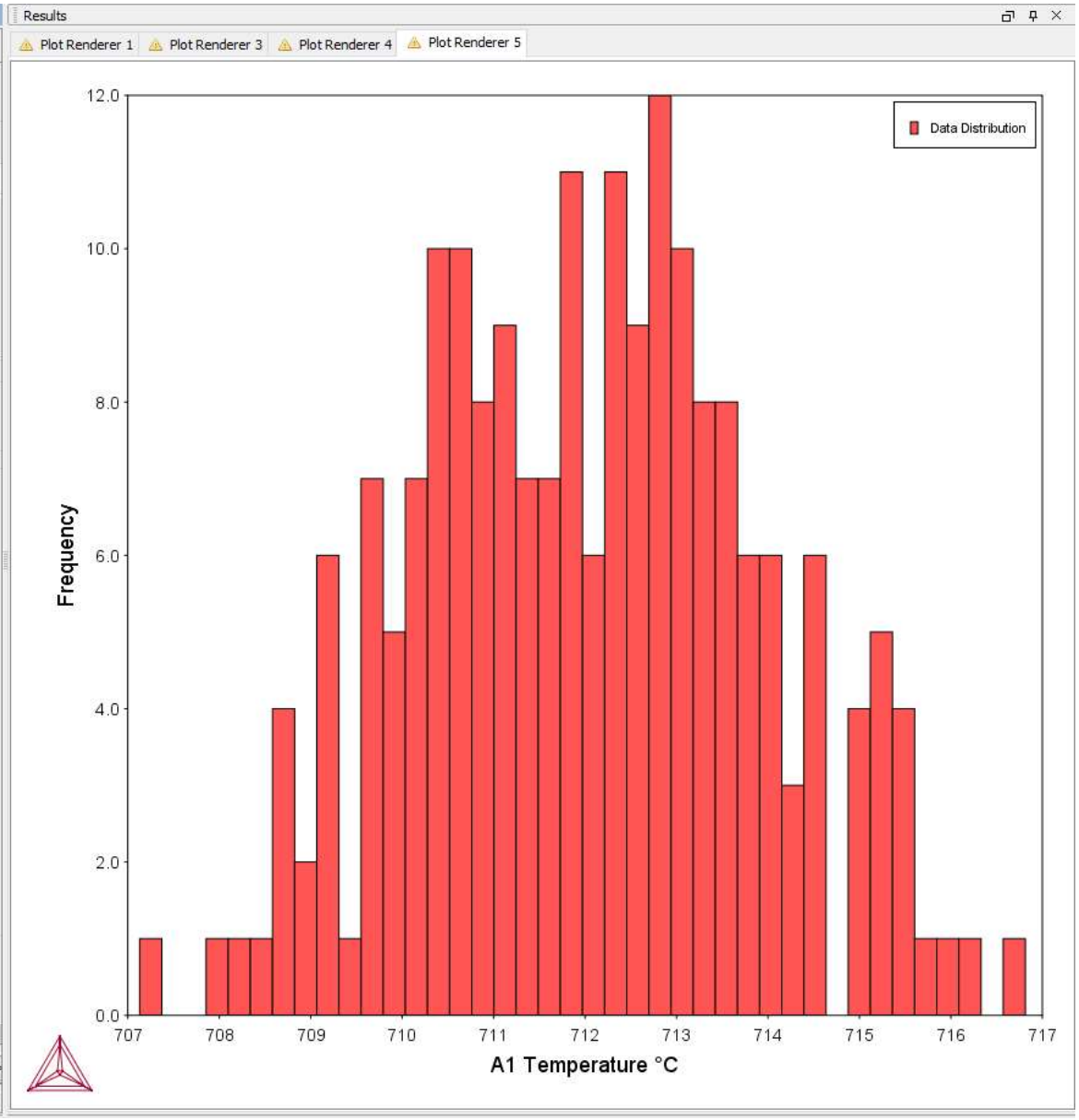
Examples in this category include e.g.

- ❑ Modifying the flux compositions to lower liquidus
- ❑ Predicting intermixing between alloy and filler material
- ❑ Looking at the influence of alloy additions to welded material microstructure



Uncertainty / Sensitivity analysis



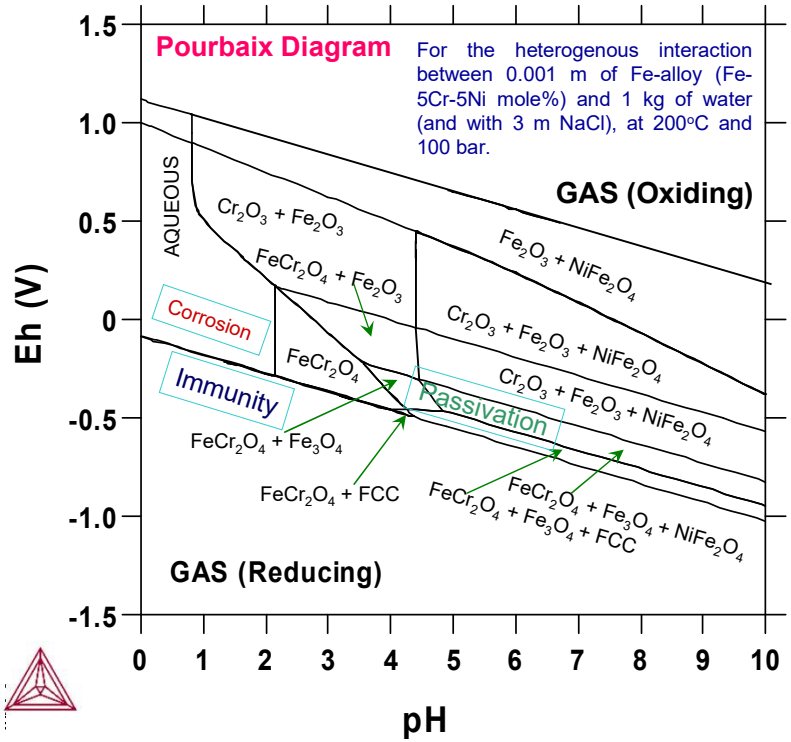


Corrosion

Thermo-Calc Software

These tools have also been applied to model different types of corrosion in alloys:

- ❑ High-temperature oxidation
- ❑ Salt corrosion
- ❑ Aqueous corrosion



Pourbaix diagram for heterogeneous interaction between 0.001 m of steel [Fe-5Cr-5Ni mole%] and 1 kg of water (and with 3 m NaCl), at 200 °C and 100 bar.

S-Eq 2: γ + γ’ in Ni Superalloy CMSX-2 at 850°C.

Some definitions

Thermo-Calc Software

System: The region of interest which can be closed or open to the exchange of matter, heat and work to its surroundings.

Phases: A region in the system which is uniform in composition and temperature at equilibrium and has the same structure everywhere.

Equilibrium State: A state stable against internal fluctuations in a number of variables.

Gibbs Phase Rule: States that the number of degrees of freedom in a system is equal to the number of components in the system minus the number of stable phases plus 2 (temperature and pressure).

Components: The smallest possible division of matter required (or sometimes chosen) to describe a given phase.

Constituents: The species a phase is made up from. In the case of phases with more than one sublattice, they will determine the composition dependence of the properties of the phase and can reflect additional internal degrees of freedom.

Species: Are the collection of all constituents for the phases in a given system and can be elements, molecular aggregates, charged or neutral.

Status of phases

Thermo-Calc Software

Entered / Selected

The phase participates in the equilibrium calculation. Default for most phases.

Suspended / De-selected

The phase does not participate in the equilibrium calculation. A suspended or dormant phase can however be used as a reference phase for G.

Dormant

The phase does not participate in the equilibrium calculation, but the driving force for precipitating the phase is calculated.

Fixed

It is a requirement that the phase is stable in the equilibrium together with at least one more phase.

Ex. Calculate the liquidus temperature of a metallic alloy.
Set the liquid as **fixed** to 1 mole (if the system size is 1 mole)

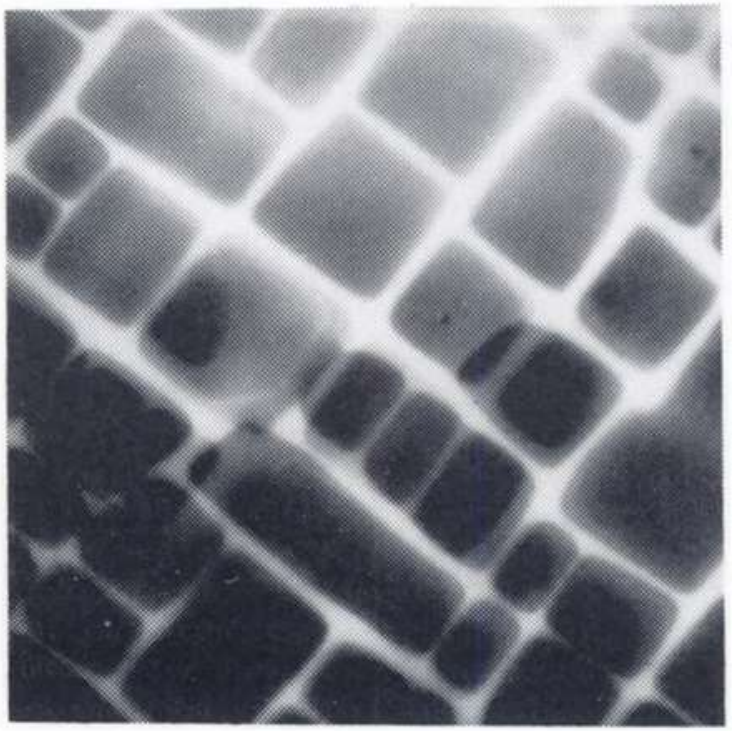
Single Equilibrium, Example 2

Thermo-Calc Software

γ-γ’ phase equilibrium in Ni Superalloy CMSX-2 at 850°C:

- Ni-12.21Al-1.25Ti-9.22Cr-5.08Co-1.99Ta-2.61W **at**.%

at%	Al	Ti	Cr	Ni	Co	Ta	W
Measured Matrix phase	3.1	0.6	25.5	59.6	8.6	0.1	2.5
Calculated γ phase	?	?	?	?	?	?	?
Measured Precipitates	16.7	3.0	2.4	70.5	3.2	3.0	2.4
Calculated γ’ phase	?	?	?	?	?	?	?



Which FCC_L12 is the gamma prime?

Blavette, D. et al. "AN ATOM-PROBE STUDY OF SOME FINE-SCALE MICROSTRUCTURAL FEATURES IN Ni-BASED SINGLE CRYSTAL SUPERALLOYS." *Superalloys, 1988 305-314.*

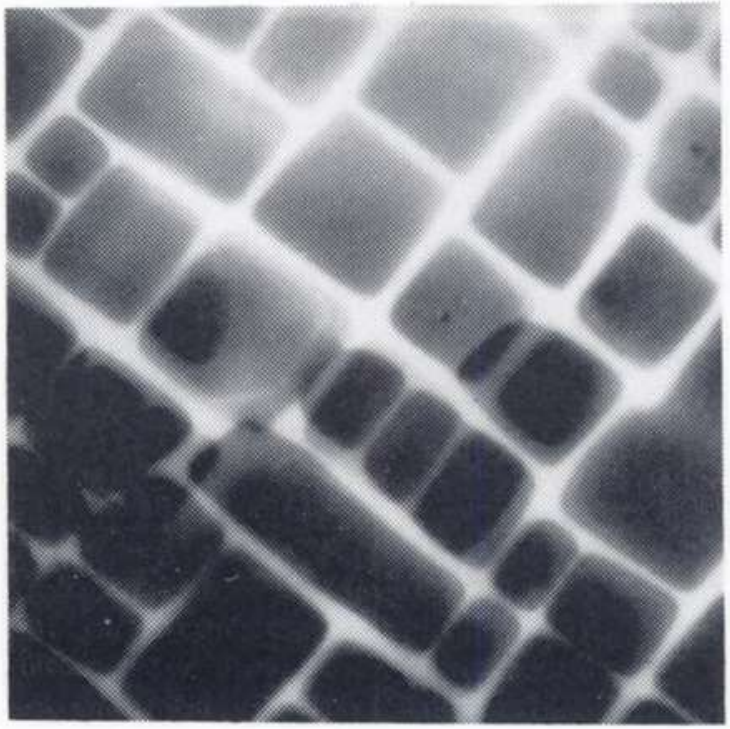
Single Equilibrium, Example 2

Thermo-Calc Software

γ-γ’ phase equilibrium in Ni Superalloy CMSX-2 at 850°C:

- Ni-12.21Al-1.25Ti-9.22Cr-5.08Co-1.99Ta-2.61W **at**.%

at%	Al	Ti	Cr	Ni	Co	Ta	W
Measured Matrix phase	3.1	0.6	25.5	59.6	8.6	0.1	2.5
Calculated γ phase	4.3	0.2	21.6	59.5	10.4	0.2	3.9
Measured Precipitates	16.7	3.0	2.4	70.5	3.2	3.0	2.4
Calculated γ’ phase	15.1	1.7	4.7	70.6	3.1	2.7	2.1



Which FCC_L12 is the gamma prime?

-- the second in the table, x(Ni)=0.706 (close to 0.75, Ni_3Al)

Blavette, D. et al. "AN ATOM-PROBE STUDY OF SOME FINE-SCALE MICROSTRUCTURAL FEATURES IN Ni-BASED SINGLE CRYSTAL SUPERALLOYS." *Superalloys, 1988 305-314.*

Thermo-Calc Software

Thermo-Calc Day 1

9:00	S-Eq 1: Stainless steel 2205.
9:30	Introduction to Thermo-Calc and CALPHAD-based software tools.
10:00	S-Eq 2: Ni superalloy CSMX-2.
10:25	**Q & A**
10:40	S-Eq 3: Stable and metastable phases in Al-Cu.
11:00	Step 1: Ni alloy Nimonic 263.
11:25	Step 2: Slag calculation, changing components.
11:45	Q & A
12:00	Handing out home assignment.

S-Eq = Single-Equilibrium Calculation

Step = One-axis Step Calculation

Thermo-Calc Software

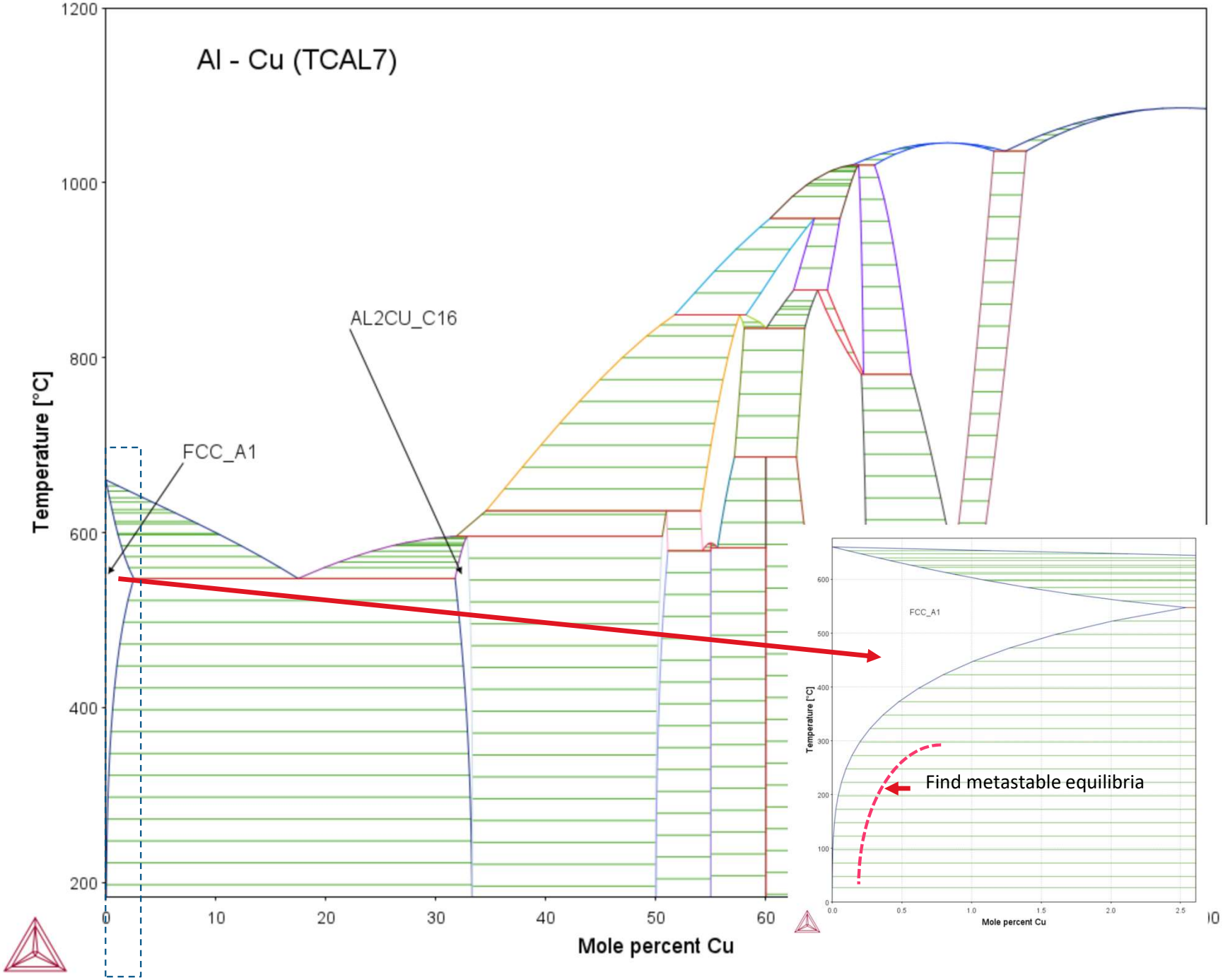
Questions

&

Answers

S-Eq 3: Al-Cu Solvus temperatures for stable and meta-stable phases.

Single Equilibrium, Example 3



Single Equilibrium, Example 3

Thermo-Calc Software

Calculate Al-Cu (Al) solvus temperatures for θ, θ ', θ '' (or GPII zones)

At.%	Phase	Temperatures from literature (°C)	Temperatures from calculation
Al-1Cu	Θ''	200 [1957Bet]	?
Al-1.5Cu	Θ'	400 [1934Mat]	?
Al-1Cu	Θ	450 [1973Hor]	?

Θ is the stable Al_2Cu phase in the binary phase diagram Al-Cu.

K. Matsuyama, Kinzoku no Kenkyu. 11 (1934) 461-490.
R. H. Beton, Beton, E.C. Rollason, J. Inst. Met. 86 (1957) 77-84.
H. Hori, K. Hirano, J. Jpn. Inst. Met. 37 (1973) 142-148.

Fix phase

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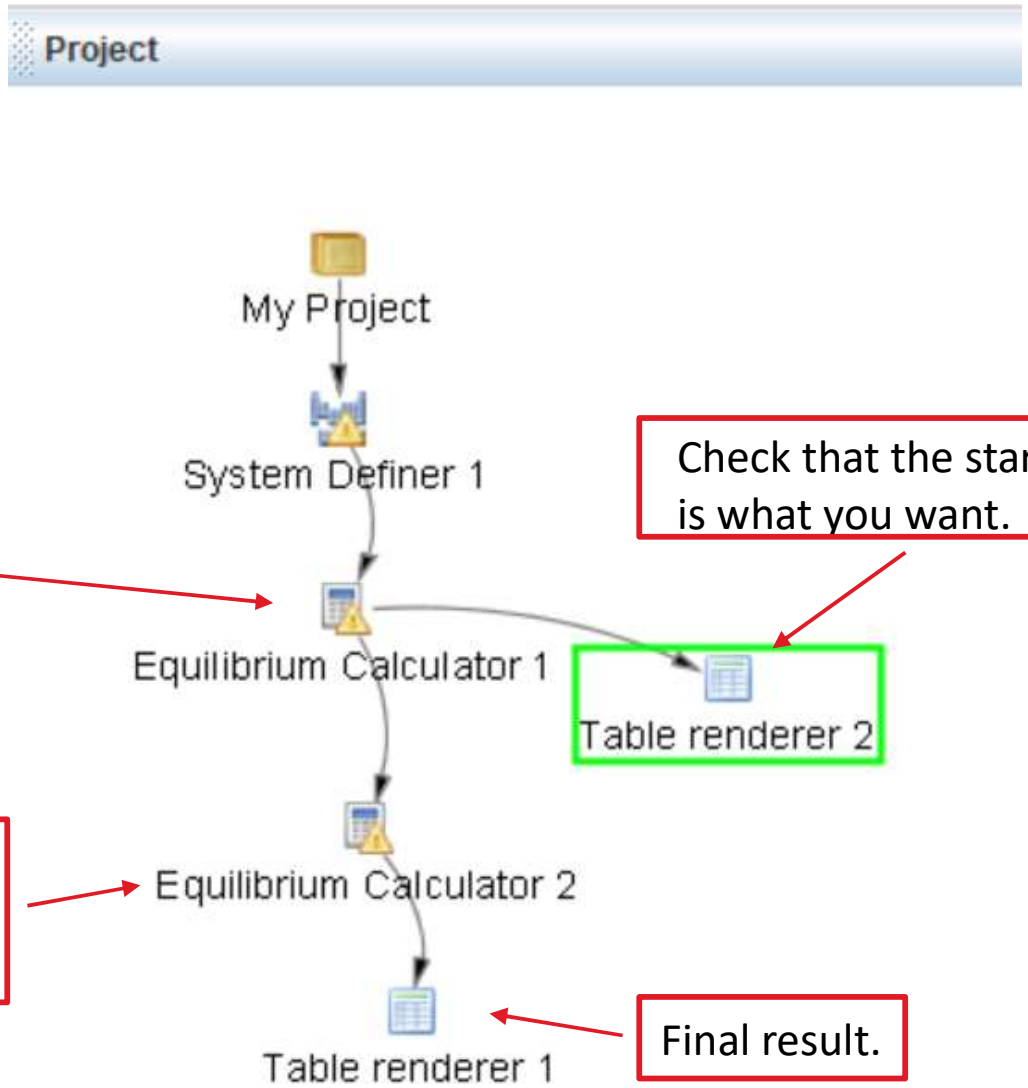
Setting a phase status fix with the value of 0 or 1 is a way to identify a point on a phase diagram line in a single-equilibrium calculation. This could be for instance a liquidus or solidus temperature.

Setting a phase fix takes up one degree of freedom, i.e. it is equal to setting a condition. The fix condition is often a more difficult condition to find the equilibrium for than just using conditions on the standard state variables, T, N, W(..) etc. It can be very dependent on start values.

Because of this it is recommended to use a start value when setting phases fix. This is achieved in Graphical mode by having two Equilibrium Calculations in sequence, see next slide.

The fix status can also be used for one-axis step calculations.

Fix phase



Start value calculation: normal conditions, if possible close to expected result.

Check that the start value is what you want.

Change one of the conditions in the first Equilibrium Calculator to a FIX phase.

Final result.

Single Equilibrium, Example 3

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Calculate Al-Cu (Al) solvus temperatures for θ, θ ', θ '' (or GPII zones)

At.%	Phase	Temperatures from literature (°C)	Temperatures from calculation
Al-1Cu	Θ''	200 [1957Bet]	198.1
Al-1.5Cu	Θ'	400 [1934Mat]	398.2
Al-1Cu	Θ	450 [1973Hor]	446.5

K. Matsuyama, Kinzoku no Kenkyu. 11 (1934) 461-490.
R. H. Beton, Beton, E.C. Rollason, J. Inst. Met. 86 (1957) 77-84.
H. Hori, K. Hirano, J. Jpn. Inst. Met. 37 (1973) 142-148.

Things to think about before making a calculation (or before evaluating the result)

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What is the most suitable database?

Should I suspend any phases?

Do I need to append any databases? (i.e. for the gas phase)?

Overall how does my calculation relate to equilibrium and what is happening in the ‘real world’?

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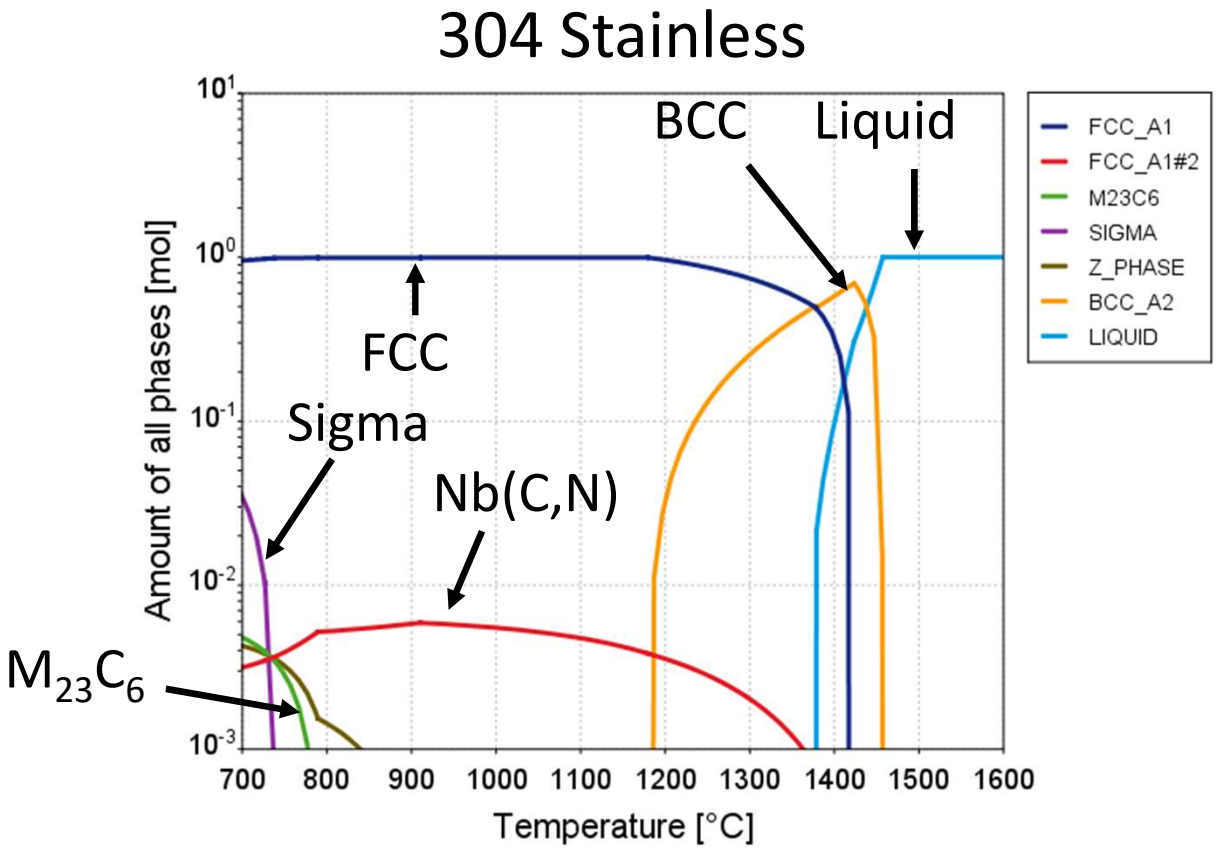
One Axis Step Calculations (Property Diagrams)

Property diagrams

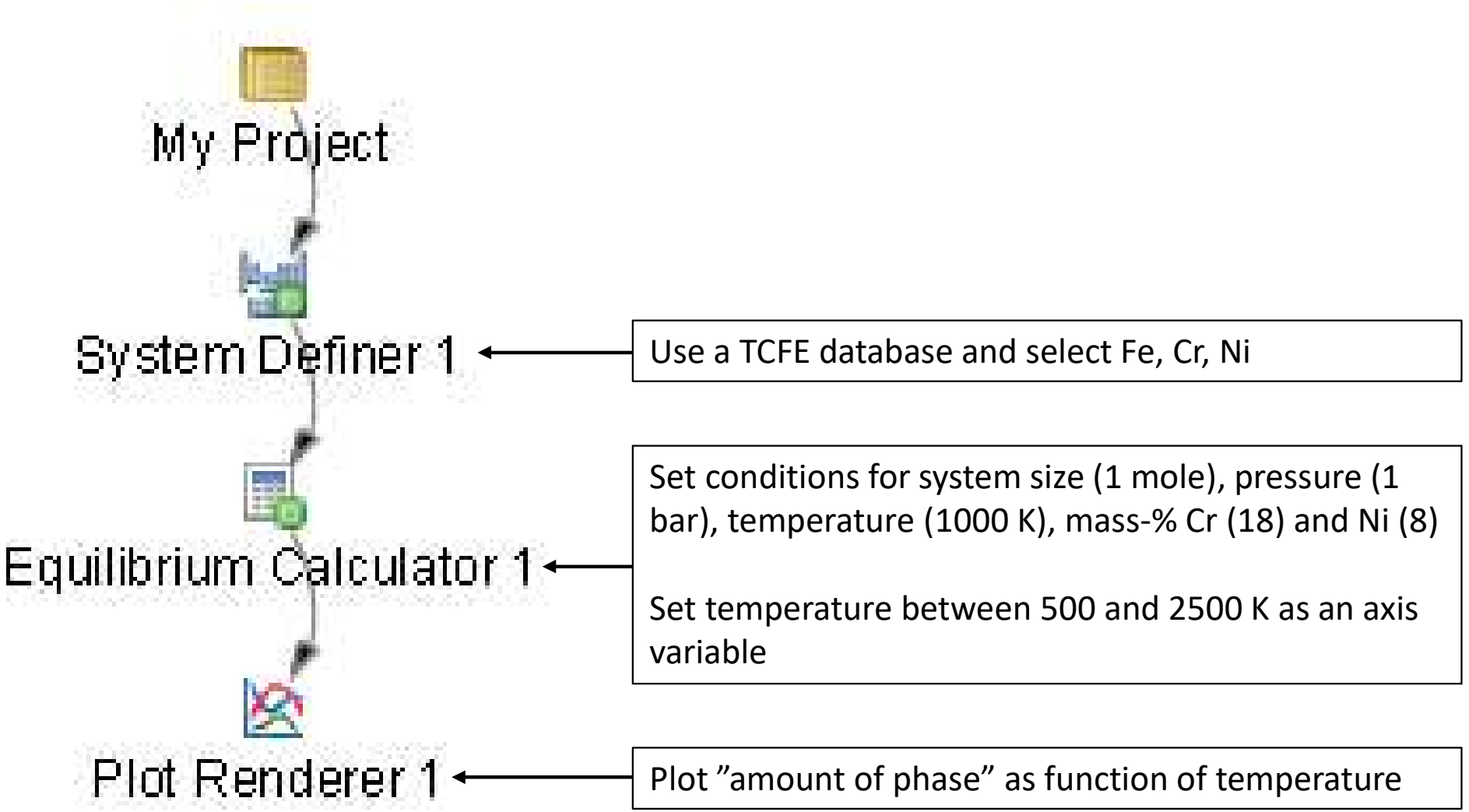
- Vary one thermodynamic state variable (e.g. temperature or composition of one alloying element).
- Plot or tabulate a dependent property as a function of the variable (e.g. phase fractions, phase compositions, enthalpy.
- Often referred to as ”One axis” or ”Step” calculations.



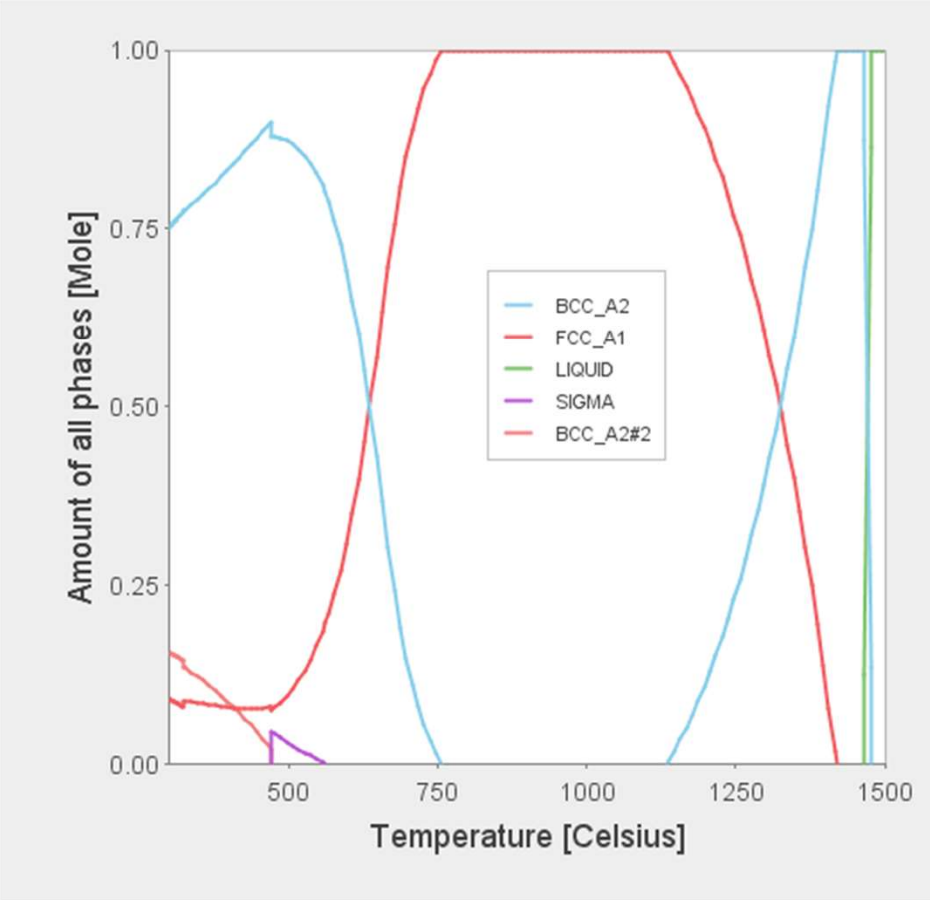
Property diagram

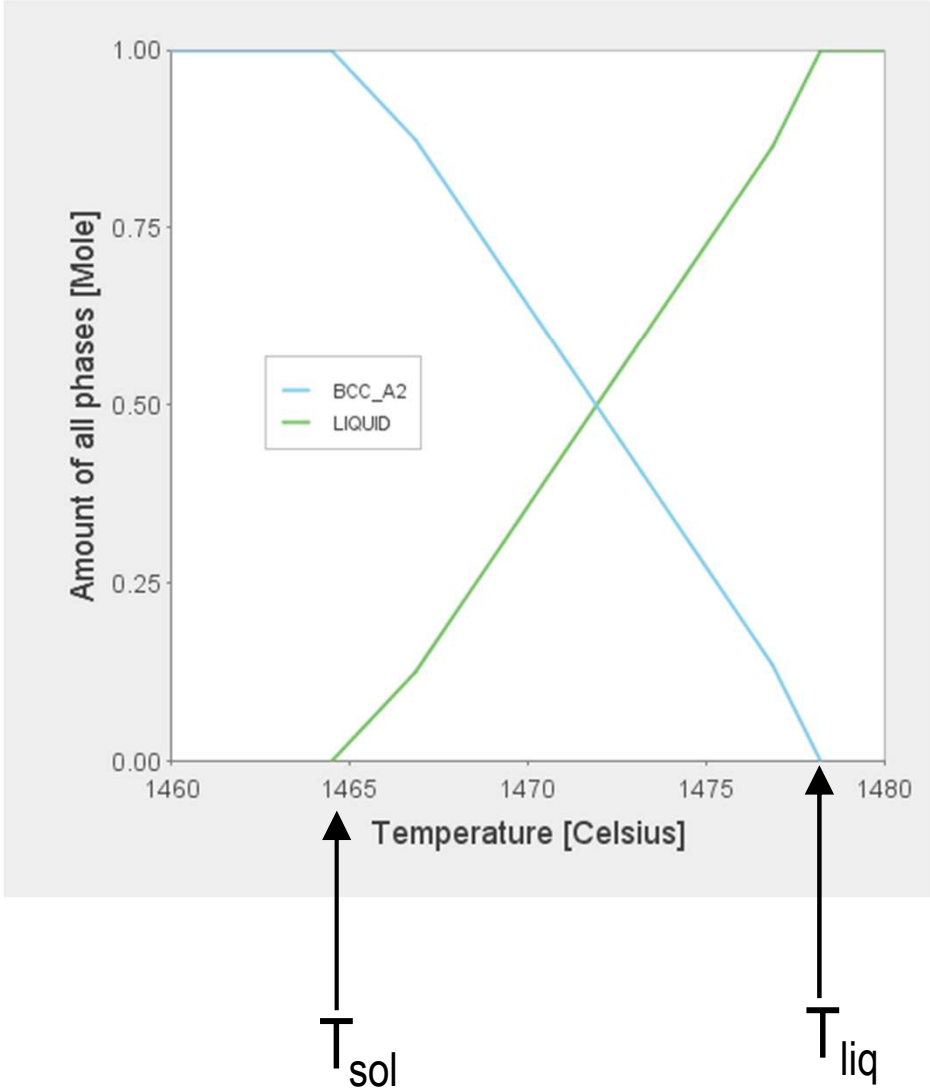
Step in one variable

Ex: Calculate the phase fractions as function of temperature for an 18-8 stainless steel



Phase fractions as a function of temperature





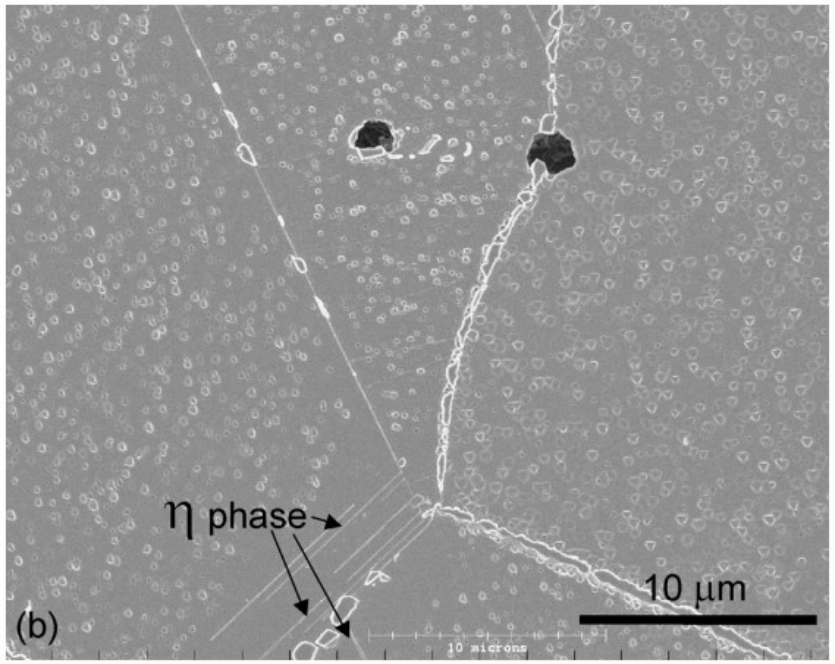
Examples of variables in property diagrams

- Thermodynamic variables:
  - Activities
  - Enthalpies
  - Heat Capacities (C_p)
- Equilibrium fraction of phases
- Equilibrium composition in one or many phases
- Density and thermal expansivity
- Thermal or electric conductivity/resistivity
- Viscosity or surface tension of the liquid phase
- Yield strength
- User defined functions

Step 1: Ni alloy Nimonic 263.
Step in temperature.

Property diagrams, Step example 1

- Ni-based superalloy Nimonic 263:
  Ni -19.5Cr -20Co -2.1Ti - 0.4Al (wt-%)



Eta phase forming at expense of γ' after 1000h at 850C

Authors report after 14000 hours at 840C, all γ' transforms to eta

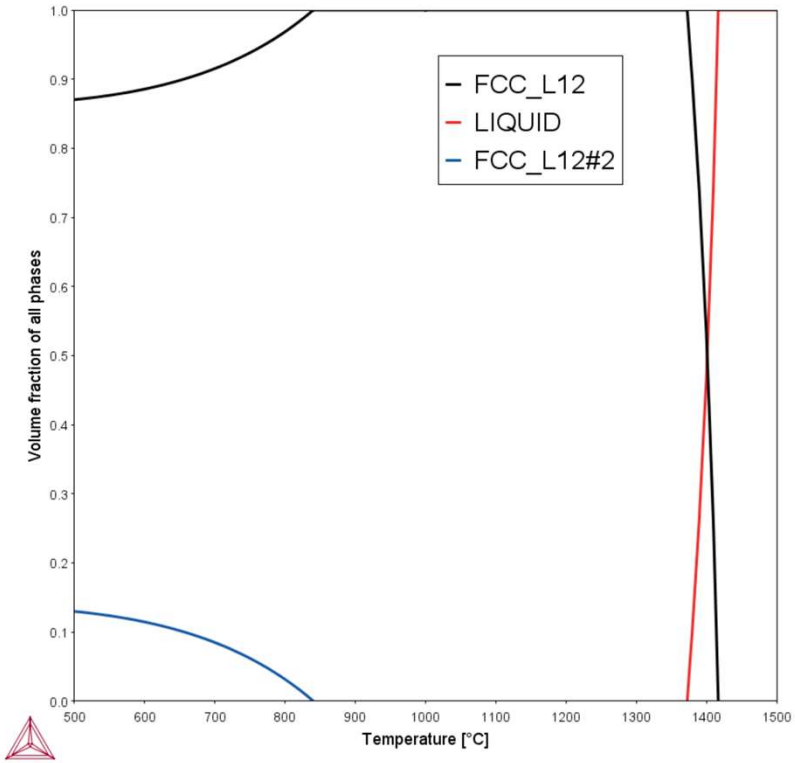
Zhao, J-C., et al., "Phase precipitation and phase stability in Nimonic 263." *Metallurgical and Materials Transactions A* 32.6 (2001): 1271-1282.

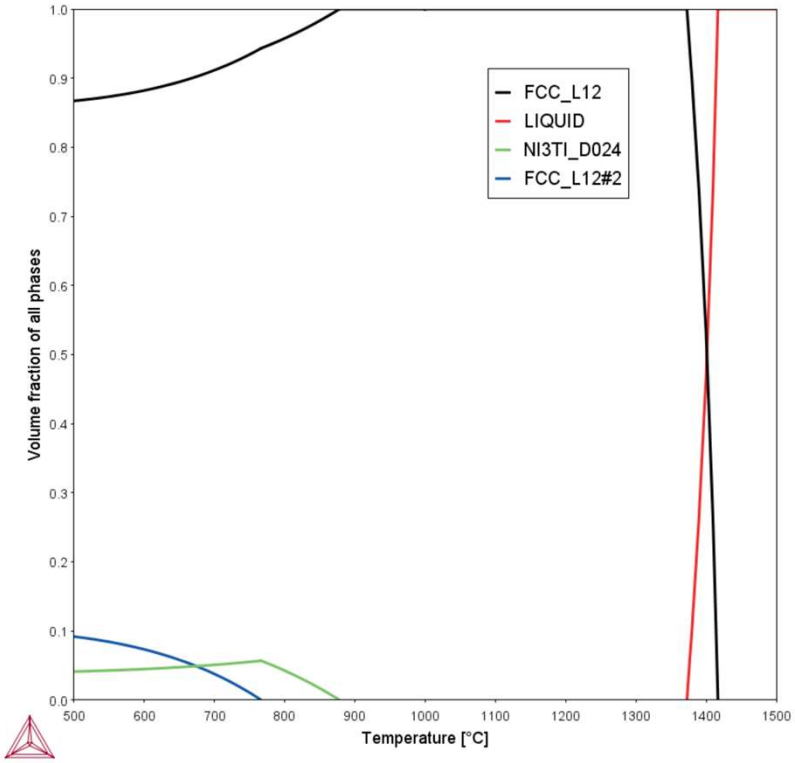
Property diagrams, Step example 1

- Ni-based superalloy Nimonic 263: Ni-19.5Cr-20Co-2.1Ti-0.4Al (wt-%)

What temperature does gamma prime form?

What temperature does gamma prime form when eta is suspended?





Step 2: Slag calculation.

Changing components for simpler set-up.

SLAG (or flux) step example 2 – define new components

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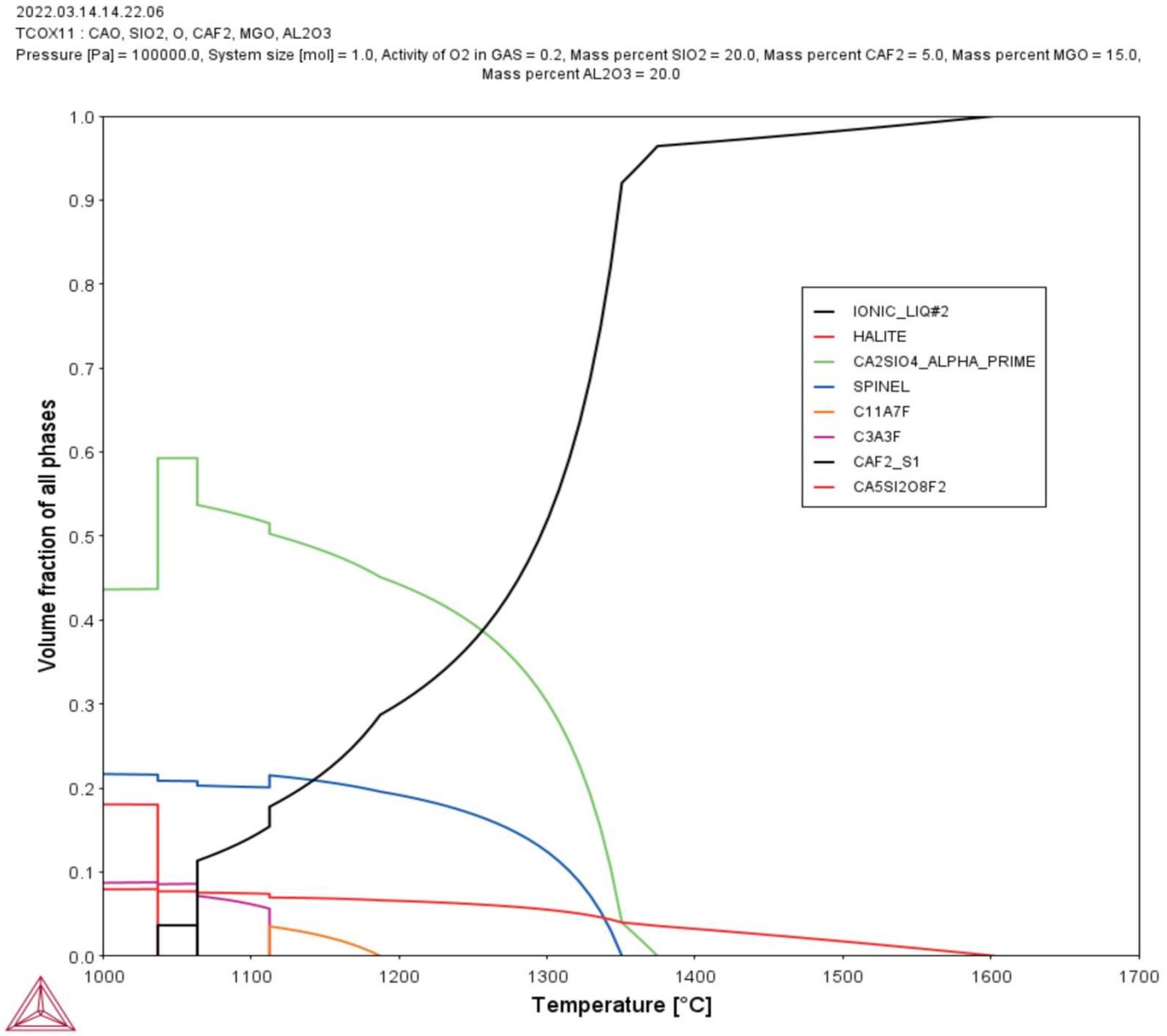
Calculate a property diagram for a simplified flux:
40 wt-% CaO
20 wt-% SiO_2
5 wt-% CaF_2
15 wt-% MgO
20 wt-% Al_2O_3

Use this composition and step in temperature.
Plot mole fraction of phases in one diagram, composition of the liquid phase in another.

SLAG (or flux) step example 2 – define new components



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Questions

&

Answers

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Home Assignment 1

Home assignment – Fixing phase

Material: Tool Steel

1) Fe - 4Cr - 8Mo - 2V - 0.3Mn - 0.3Si - 1C (wt-%)

   a) Calculate the liquidus temperature for the steel.

   b) How does the liquidus temperature change with carbon content?

More than one way to solve!

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https://download.thermocalc.com/courses/TC-Day2/