

Thermo-Calc Software

Thermo-Calc On-line Training

October 7 – 9, 2025



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 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.

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.

Course material for download

The download link for the course material is:

<https://download.thermocalc.com/training/TC-Day1/>

It contains a folder with the files:

TC-Day1.pdf pdf of all today's slides

S-Eq1-Stainless2205.tcu

S-Eq2-Ni-Alloy-850.tcu

S-Eq3-AlCu-precipitates.tcu

Step1-Nimonic-263.tcu

Step2-slag.tcu

} Project files corresponding to each
calculation example today.

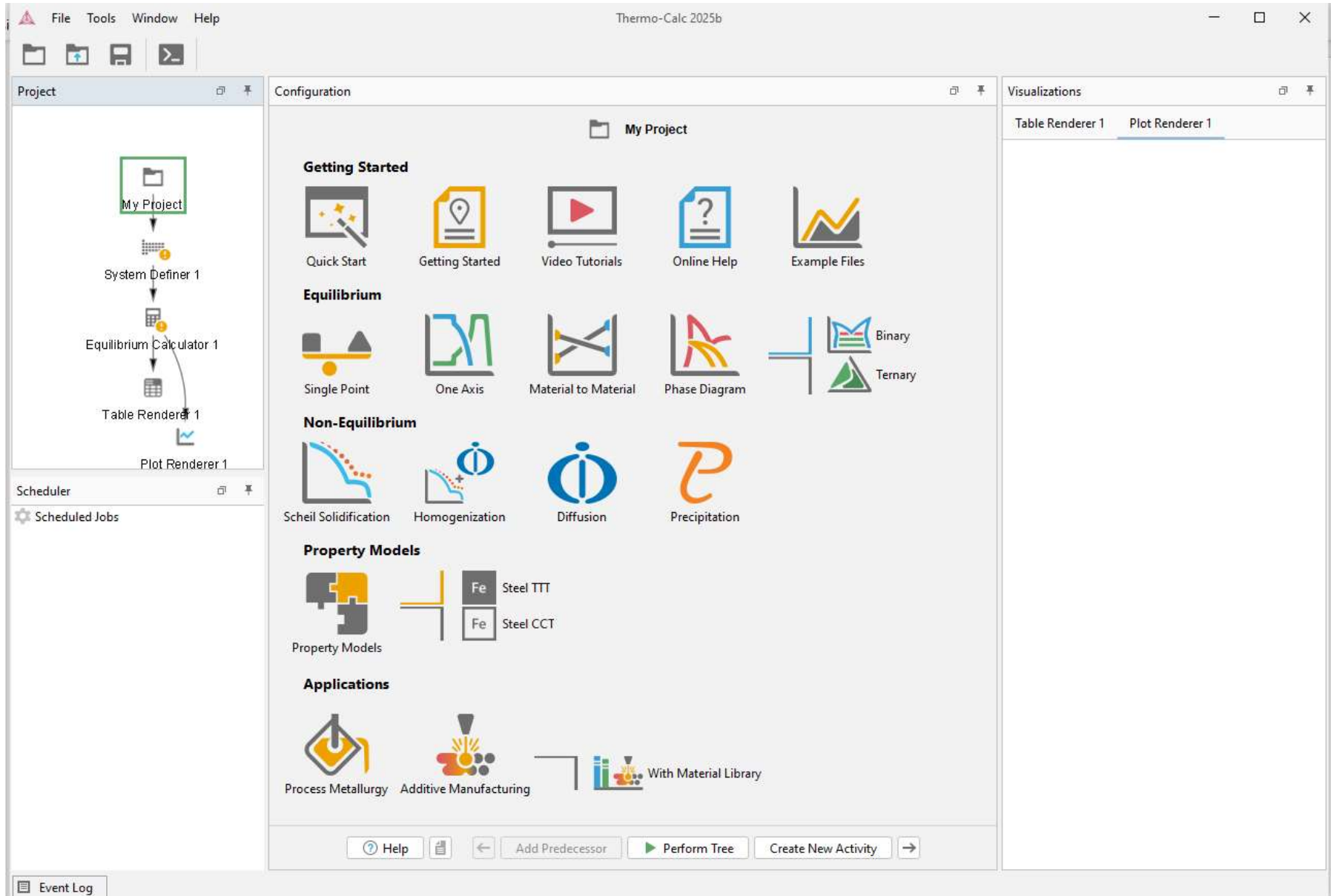
Folders for TC-Day2 and TC-Day3 are (or will be) available at

<https://download.thermocalc.com/training/TC-Day2/>

<https://download.thermocalc.com/training/TC-Day3/>

You need not read the material ahead of the course.

Overview of Thermo-Calc 2025b



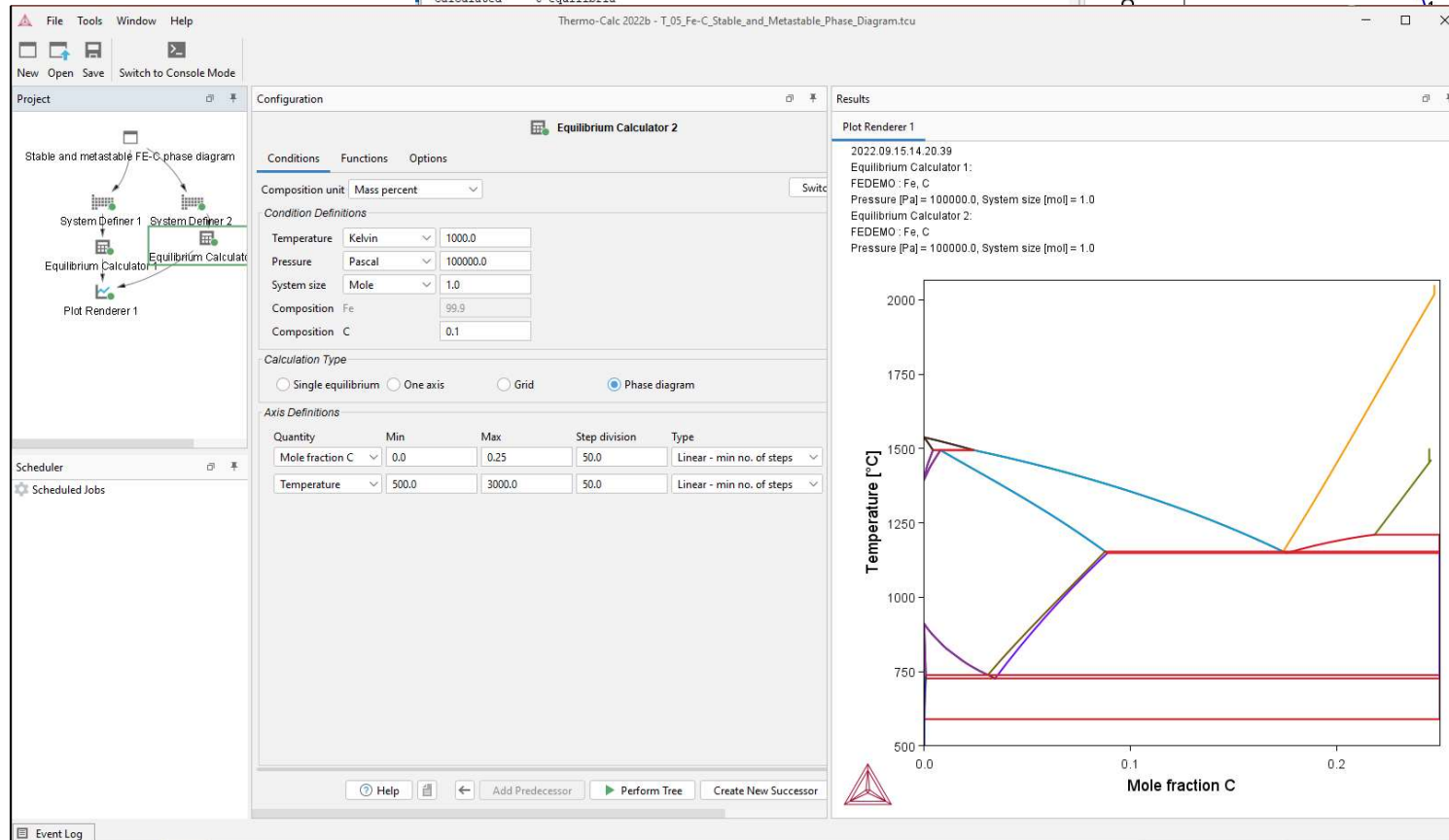
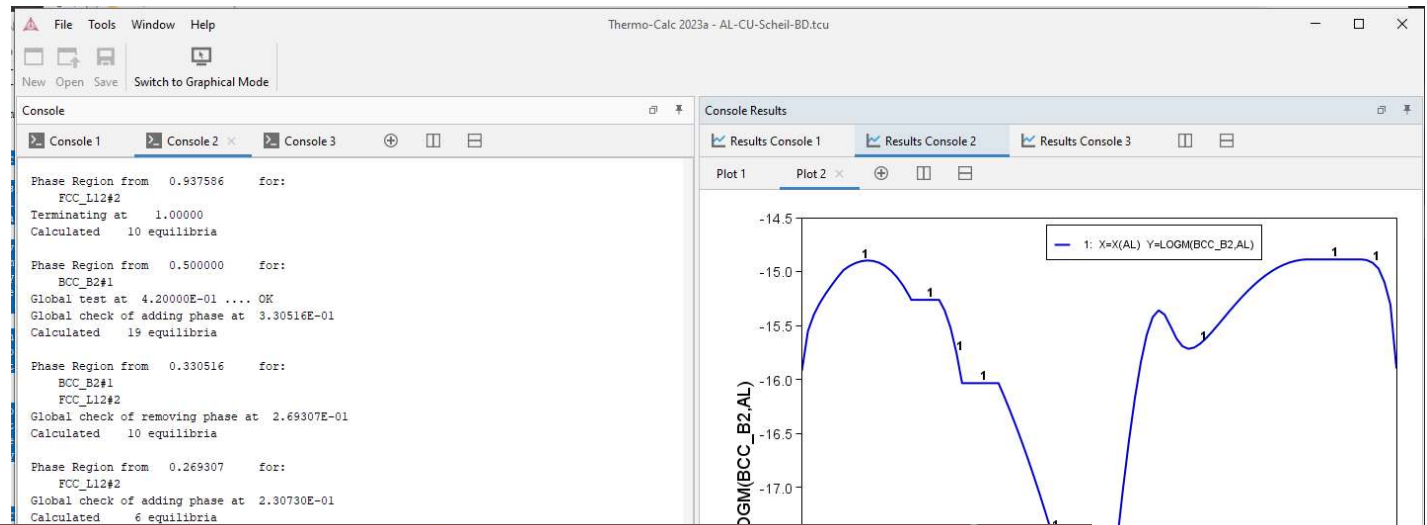
The screenshot displays the Thermo-Calc 2025b software interface, organized into several panels:

- Project Panel:** Shows a workflow diagram starting with 'My Project' (highlighted with a green box), followed by 'System Definer 1', 'Equilibrium Calculator 1', 'Table Renderer 1', and 'Plot Renderer 1'.
- Configuration Panel:** Titled 'My Project', it contains a grid of icons categorized by function:
 - Getting Started:** Quick Start, Getting Started, Video Tutorials, Online Help, Example Files.
 - Equilibrium:** Single Point, One Axis, Material to Material, Phase Diagram, Binary, Ternary.
 - Non-Equilibrium:** Scheil Solidification, Homogenization, Diffusion, Precipitation.
 - Property Models:** Property Models, Steel TTT, Steel CCT.
 - Applications:** Process Metallurgy, Additive Manufacturing, With Material Library.
- Visualizations Panel:** Contains tabs for 'Table Renderer 1' and 'Plot Renderer 1'.
- Scheduler Panel:** Labeled 'Scheduled Jobs'.
- Event Log Panel:** Located at the bottom left.

At the bottom of the Configuration panel, there is a toolbar with buttons: Help, Add Predecessor, Perform Tree, and Create New Activity.

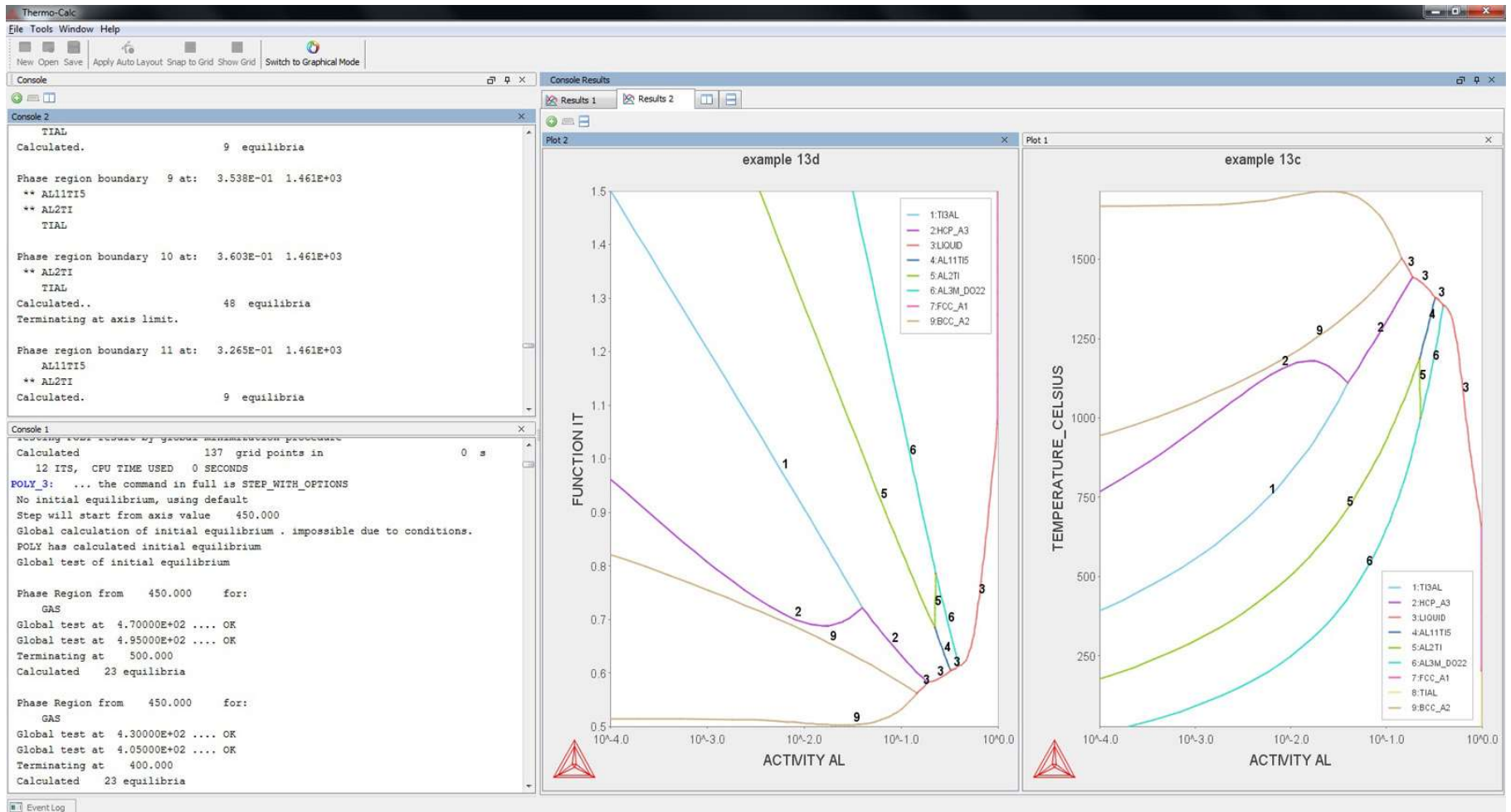
Overview of Thermo-Calc 2025b

Console Mode

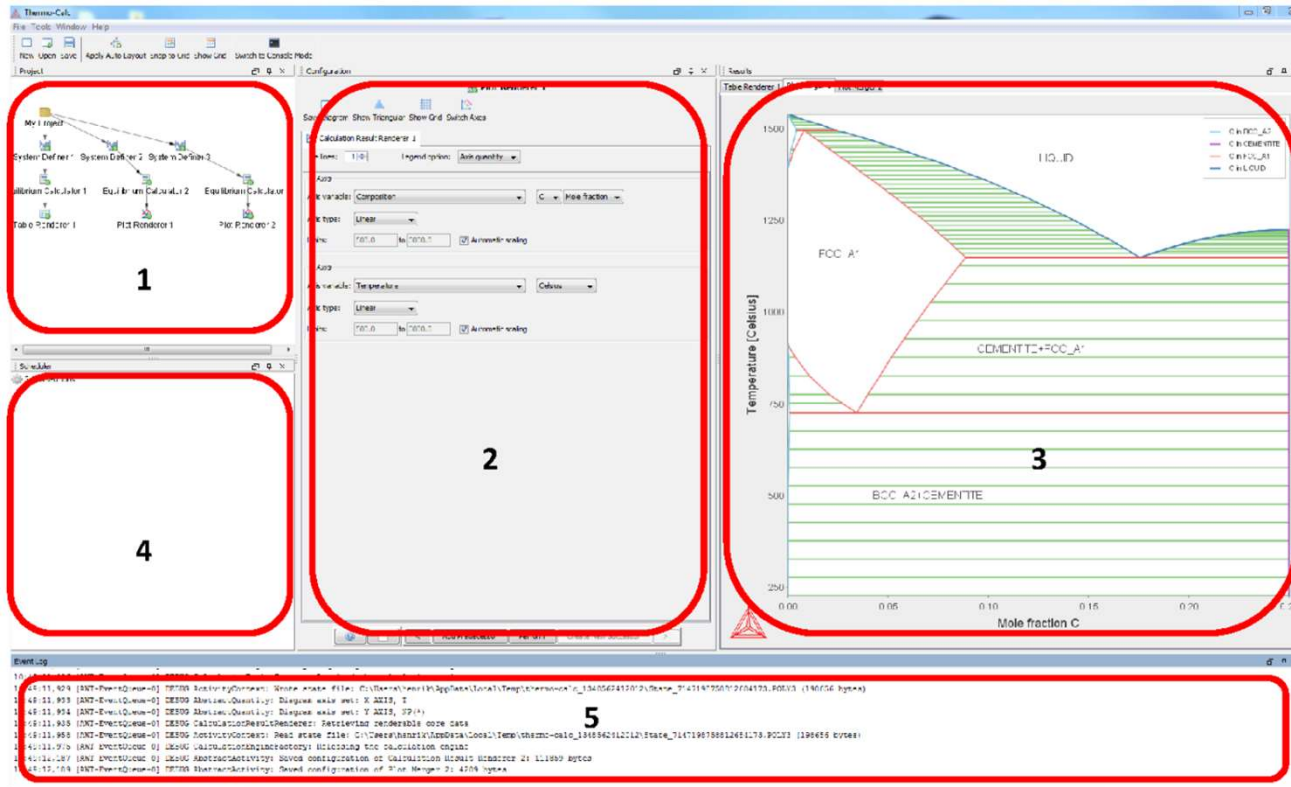


Graphical Mode

Using Console Mode



Graphical mode - GUI Layout

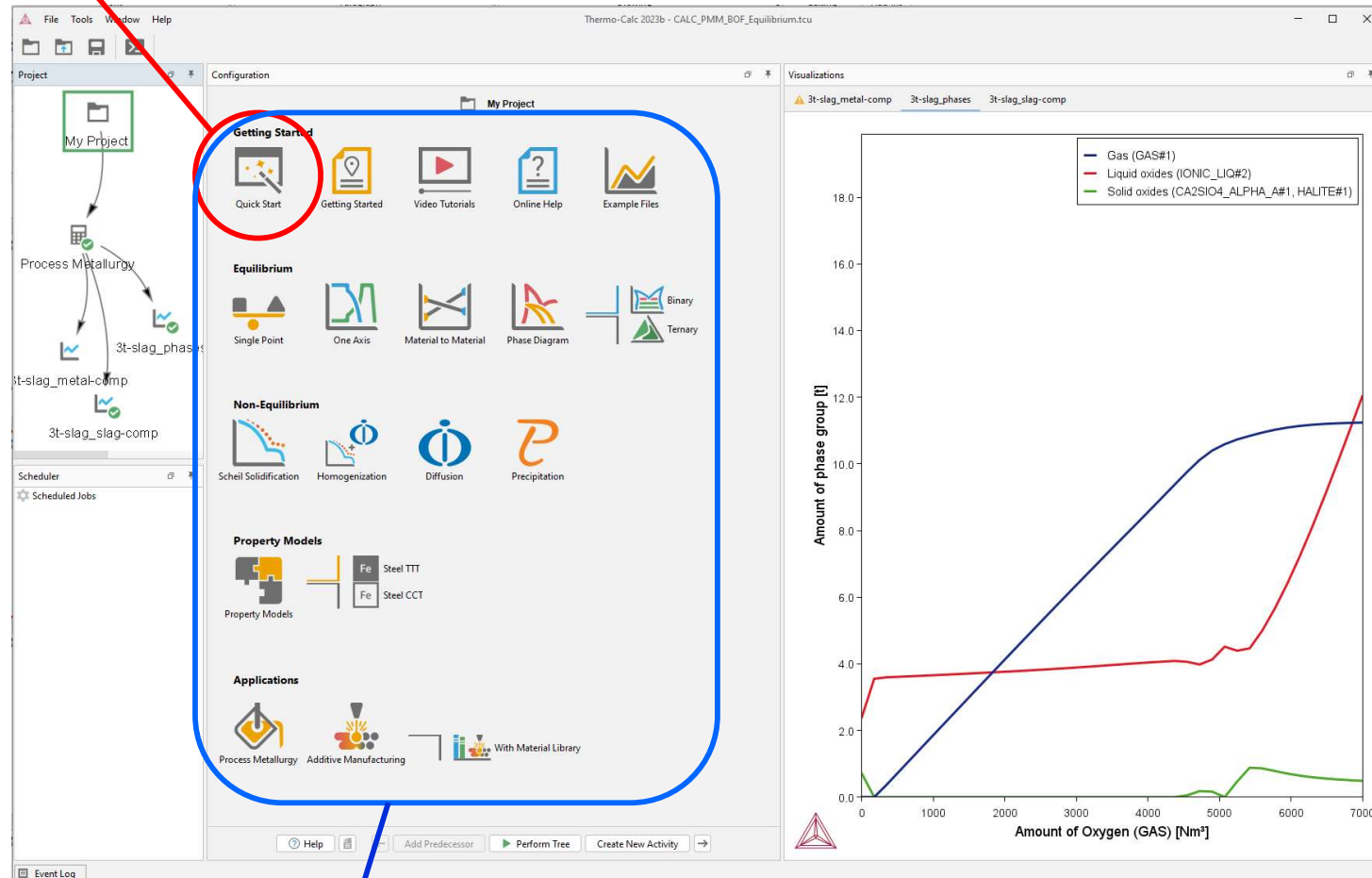


1. Project window – shows relations between defined *activities*
2. Configuration window – for configuring the selected *activity*
3. Results window – graphic and text output
4. Scheduler window – shows performed and scheduled calculations
5. Event log window – text output of progress

Getting Started

"Quick Start"

Step-by-step instructions for some common tasks



"Templates"

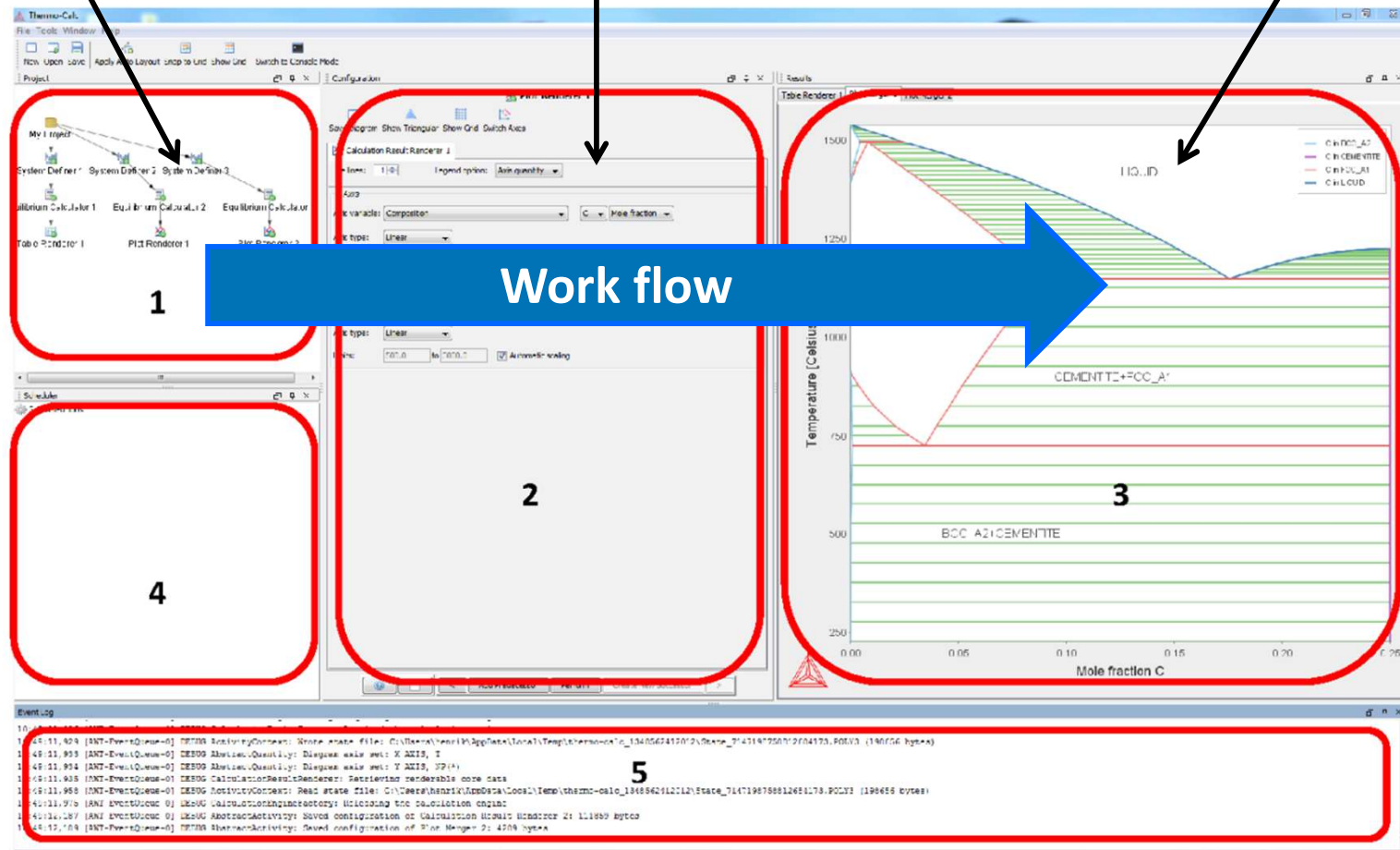
Sets up the framework for certain specific tasks

GUI layout

Set-up

Configure

Results



Single Point Equilibrium Calculations

Single Equilibrium Calculations

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				
BCC_A2#1	Moles	Mass	Volume Fraction	
	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		
FCC_A1#1	Moles	Mass	Volume Fraction	
	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

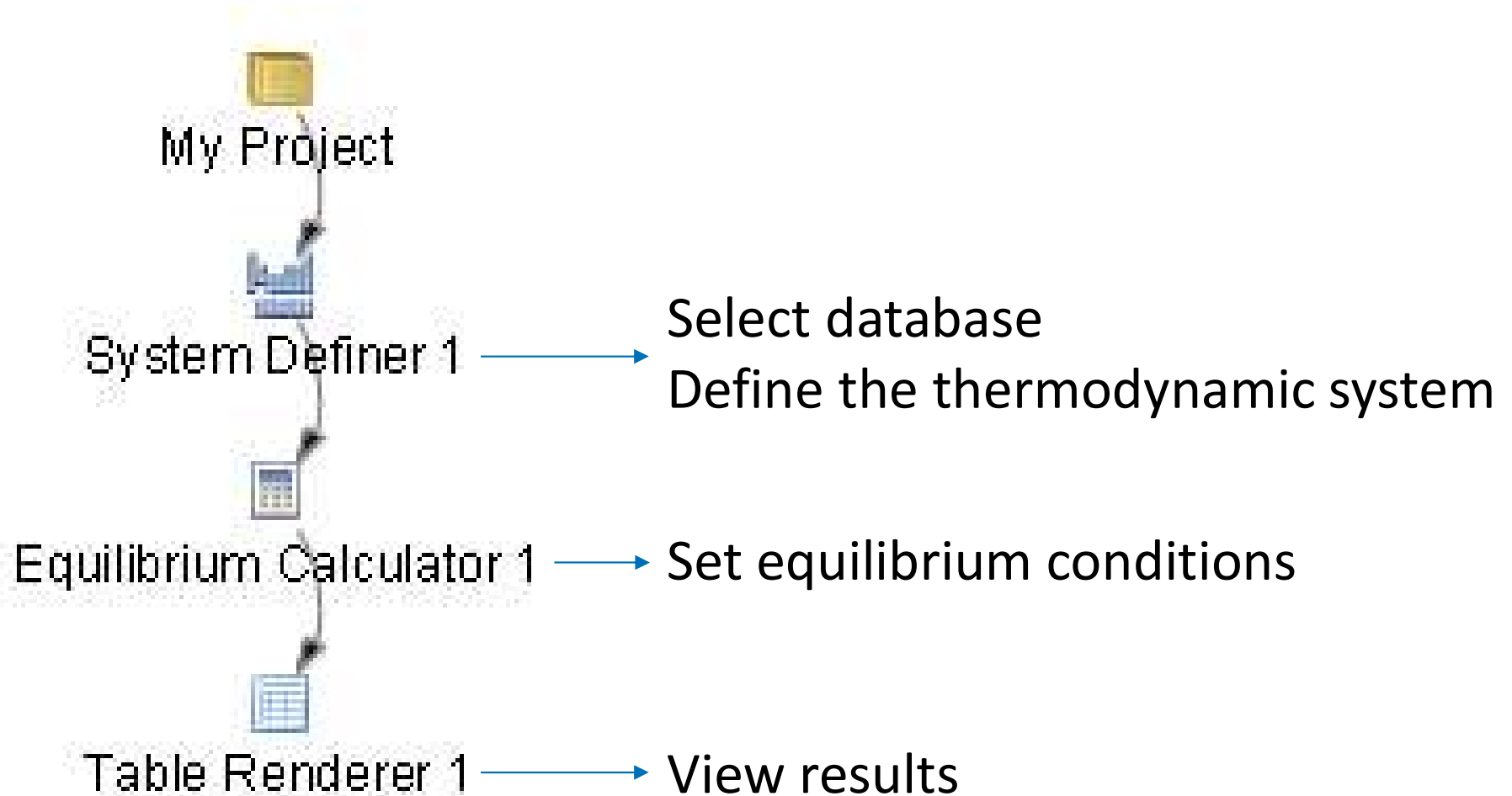
Phase Data:

Equilibrium amounts

Equilibrium compositions

The results are viewed in the Table Renderer.

General work flow

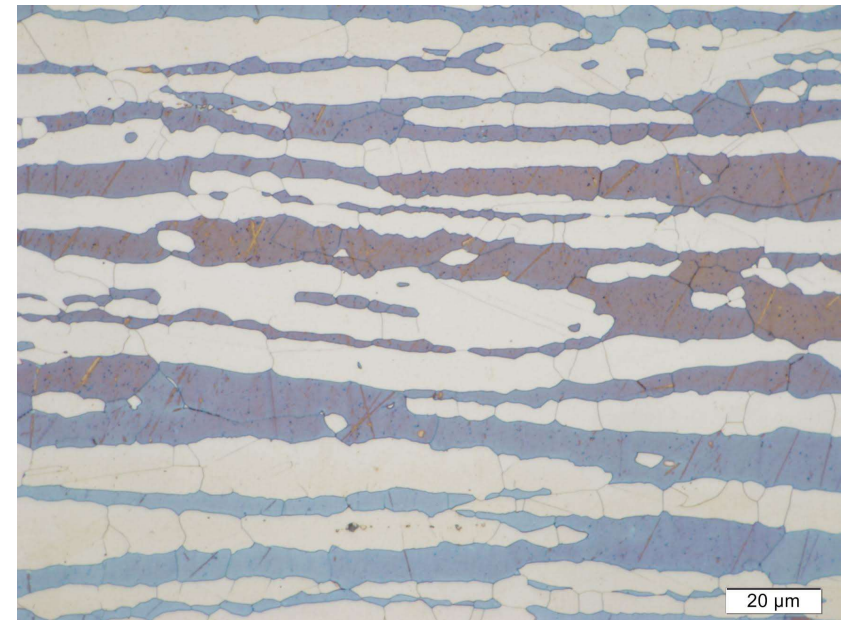
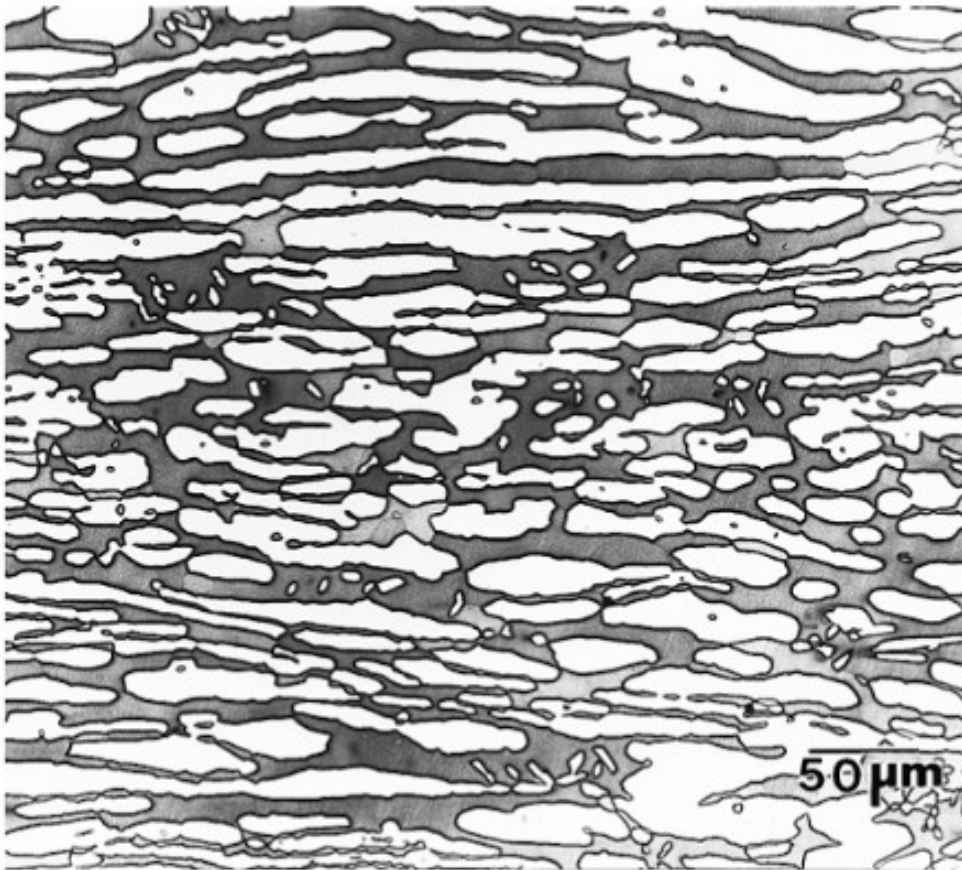


S-Eq 1: Heat treatment of duplex stainless steel 2205 at 1050 °C.

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)



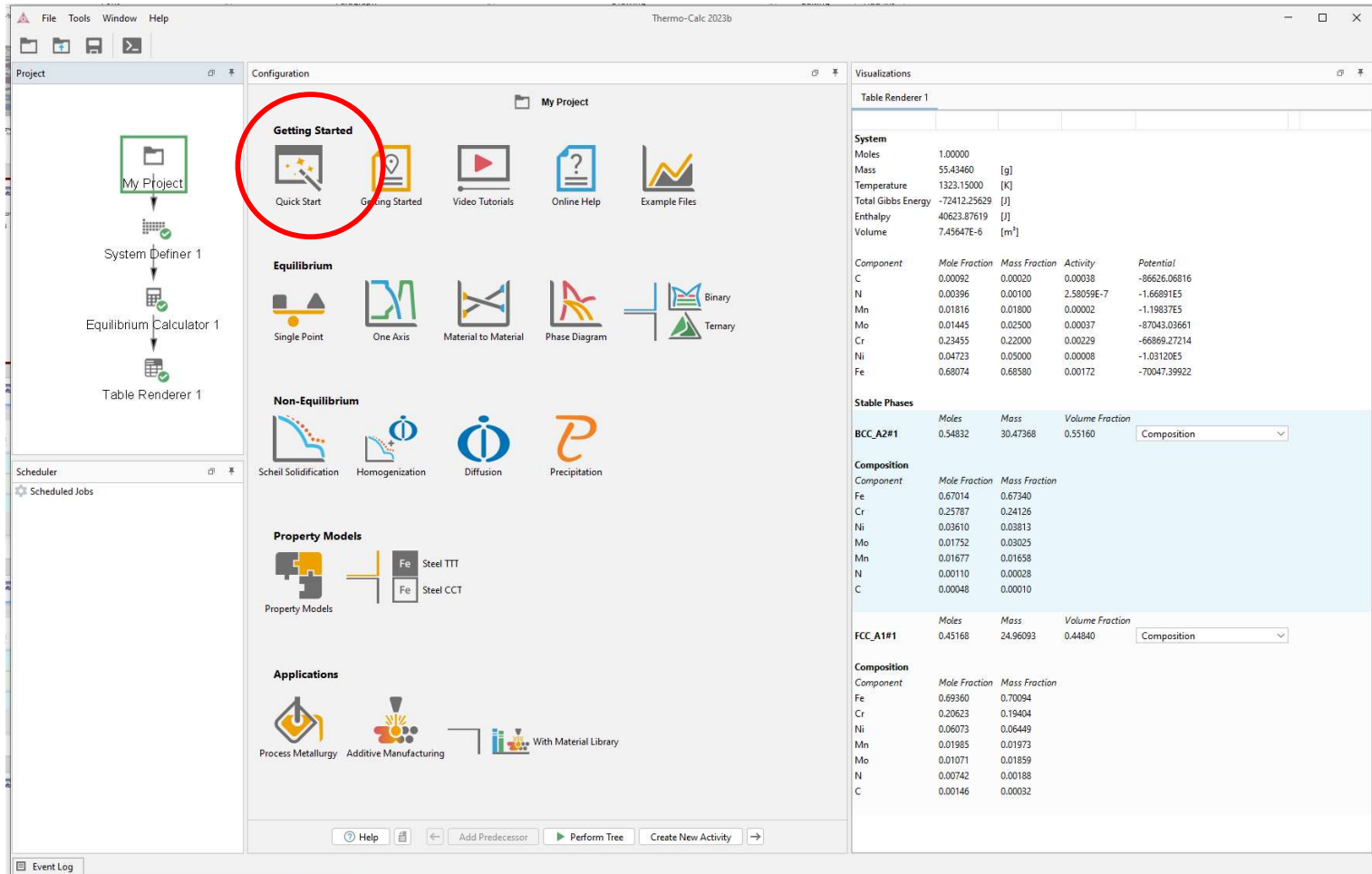
Bramfitt, Bruce L., and Arlan O. Benscoter. *Metallographer's guide: practice and procedures for irons and steels*. Asm International, 2001.

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



The screenshot displays the Thermo-Calc 2023b software interface. The 'Getting Started' icon in the 'Configuration' panel is circled in red. The interface is divided into several sections:

- Project:** A workflow diagram showing 'My Project' leading to 'System Definer 1', 'Equilibrium Calculator 1', and 'Table Renderer 1'.
- Configuration:** A central panel with various icons for calculation types: 'Getting Started' (circled), 'Quick Start', 'Video Tutorials', 'Online Help', 'Example Files', 'Equilibrium' (Single Point, One Axis, Material to Material, Phase Diagram, Binary, Ternary), 'Non-Equilibrium' (Scheil Solidification, Homogenization, Diffusion, Precipitation), 'Property Models' (Fe Steel TTT, Fe Steel CCT), and 'Applications' (Process Metallurgy, Additive Manufacturing, With Material Library).
- Visualizations:** A panel on the right showing system and composition data.

System Data:

System	Moles	Mass	Temperature	Total Gibbs Energy	Enthalpy	Volume
	1.00000	55.43460 [g]	1323.15000 [K]	-72412.25629 [J]	40623.87619 [J]	7.45647E-6 [m ³]

Component Data:

Component	Mole Fraction	Mass Fraction	Activity	Potential
C	0.00092	0.00020	0.00038	-86626.06816
N	0.00396	0.00100	2.58059E-7	-1.66891E5
Mn	0.01816	0.01800	0.00002	-1.19837E5
Mo	0.01445	0.02500	0.00037	-87043.03661
Cr	0.23455	0.22000	0.00229	-66869.27214
Ni	0.04723	0.05000	0.00008	-1.03120E5
Fe	0.68074	0.68580	0.00172	-70047.39922

Stable Phases:

Stable Phases	Moles	Mass	Volume Fraction
BCC_A2#1	0.54832	30.47368	0.55160

Composition:

Component	Mole Fraction	Mass Fraction
Fe	0.67014	0.67340
Cr	0.25787	0.24126
Ni	0.03610	0.03813
Mo	0.01752	0.03025
Mn	0.01677	0.01658
N	0.00110	0.00028
C	0.00048	0.00010

FCC_A1#1:

Component	Mole Fraction	Mass Fraction
Fe	0.69360	0.70094
Cr	0.20623	0.19404
Ni	0.06073	0.06449
Mn	0.01985	0.01973
Mo	0.01071	0.01859
N	0.00742	0.00188
C	0.00146	0.00032

Single point equilibrium

Thermo-Calc

File Tools Window Help

New Open Save Apply Auto Layout Snap to Grid Show Grid Switch to Console Mode

Project

My Project

System Definer 1

Equilibrium Calculator 1

Table Renderer 1

Scheduler

Scheduled Jobs

Event Log

Configuration

Equilibrium Calculator 1

Conditions Functions Options

Composition unit: Mass percent

Switch to advanced mode

Condition Definitions

Temperature: Celsius 1000.0

Pressure: Pascal 101325.0

System size: Mole 1.0

Composition: Cr 22.0

Composition: Ni 5.5

Composition: Mo 3.0

Composition: N 0.14

Composition: Fe 69.36

Axis Definitions

Quantity Min Max Step Division Type

Temperature [Celsius] 500.0 3000.0 50.0 Linear - no. of steps Normal

Temperature [Celsius] 500.0 3000.0 50.0 Linear - no. of steps Normal

Results

Table Renderer 1

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

FCC_A1#1 0.54634 30.24081 0.54248 Composition

Composition

Component Mole Fraction Mass Fraction

Ni 0.06457 0.06846

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FCC_A1#2 0.00000E0 0.00000E0 0.00000E0 Composition

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Add Predecessor Perform Create New Successor

Single point equilibrium

Thermo-Calc

File Tools Window Help

New Open Save Apply Auto Layout Snap to Grid Show Grid Switch to Console Mode

Project

Configuration

Equilibrium Calculator 1

Conditions Functions Options

Composition unit: Mass percent

Switch to advanced mode

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Mo 0.01361 0.02360

Scheduler

Scheduled Jobs

Event Log

My Project

System Definer 1

Equilibrium Calculator 1

Table Renderer 1

"activities"

Single point equilibrium

System

Moles	1.00000	
Mass	55.55397	[Gram]
Temperature	1273.15000	[Kelvin]
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Stable Phases

	Moles	Mass	Volume Fraction	
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Composition

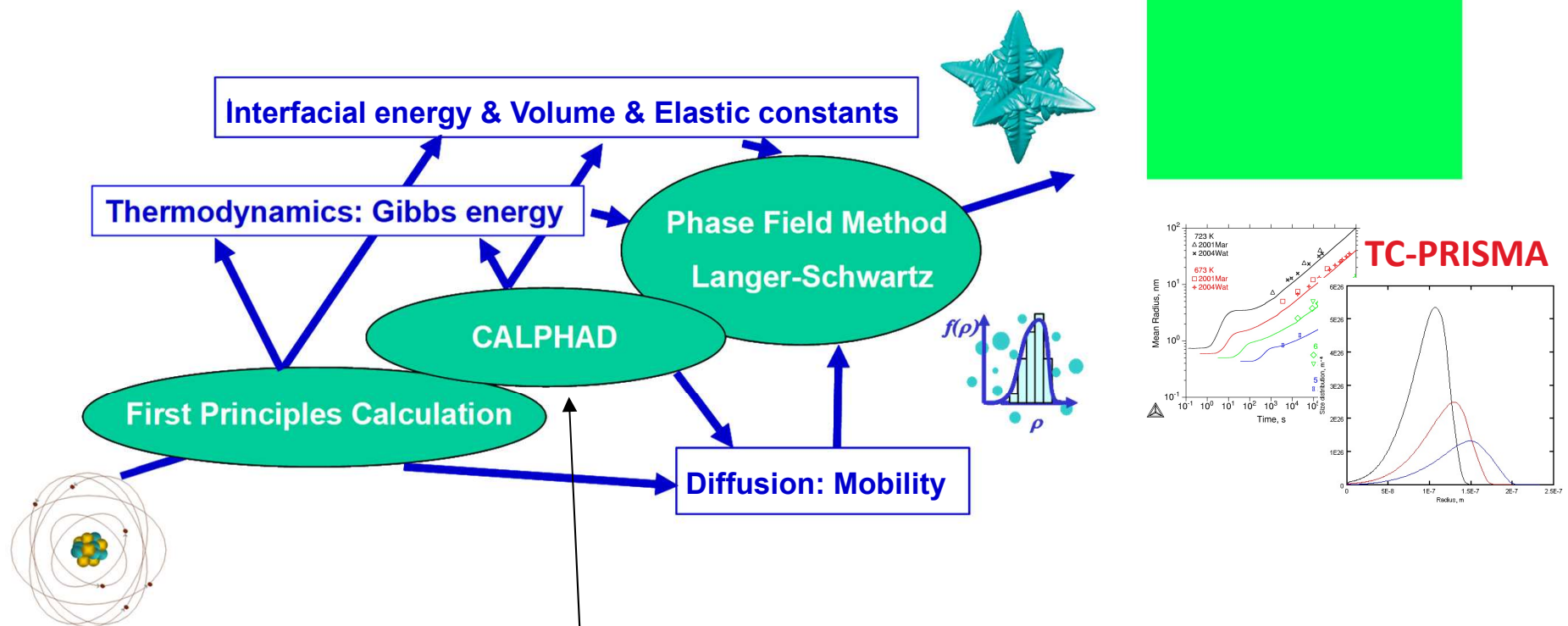
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Introduction to Thermo-Calc and CALPHAD-based software tools

Our field of operation

Towards prediction of microstructure evolution and material properties

Bridging Atoms and Microstructure



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?



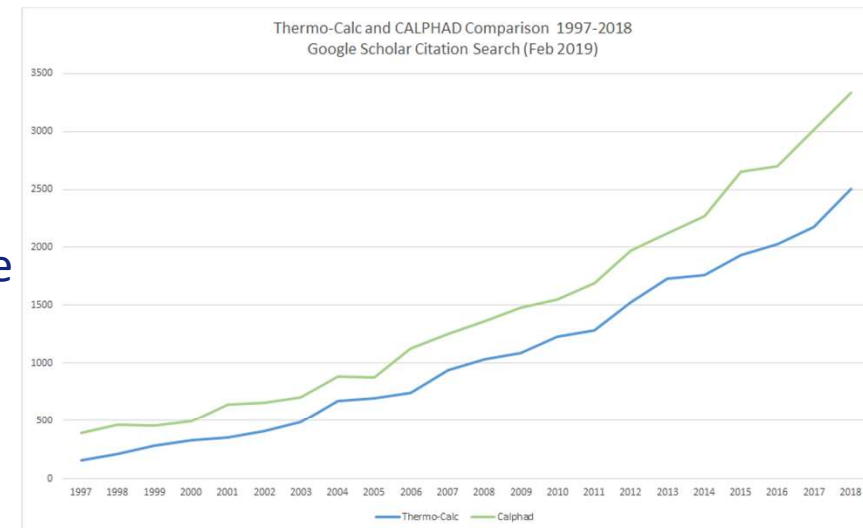
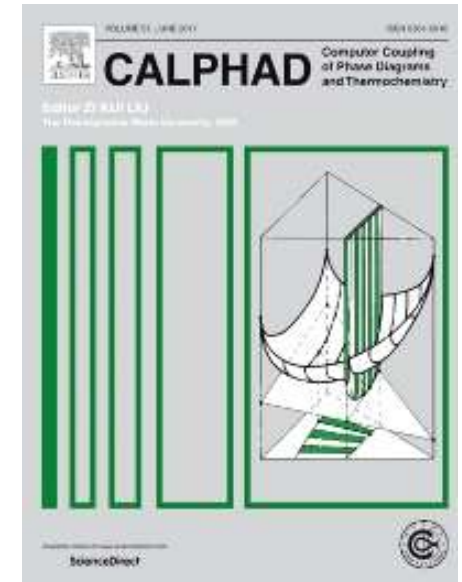
CALculation of PHase Diagrams

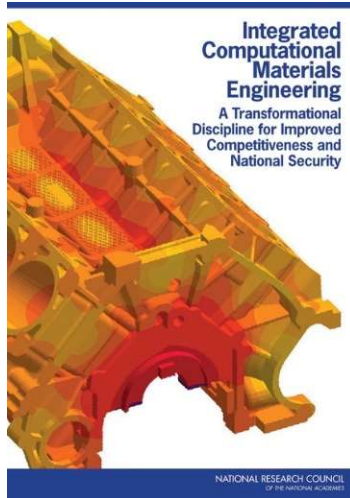
A phase based approach to modeling the underlying thermodynamics and phase equilibria of a system through a self consistent framework that allows extrapolation to multicomponent systems.

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.





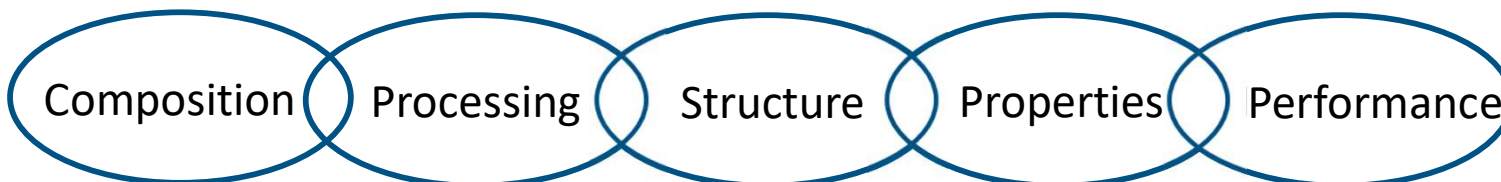
The National Academies Press, 2008

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

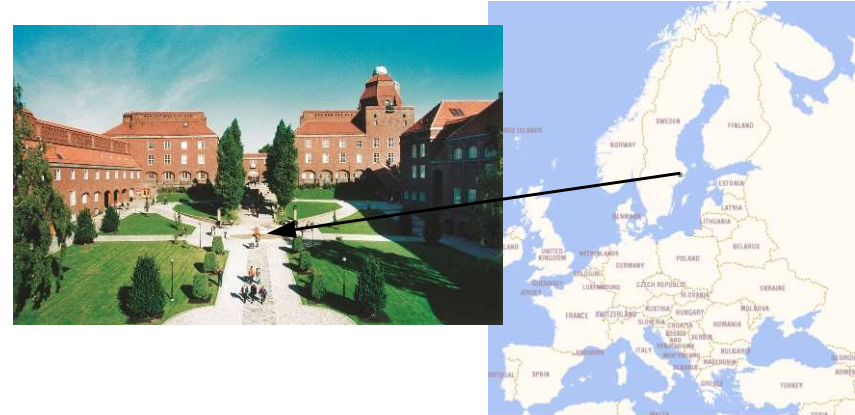
Moving beyond Materials Discovery...

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:

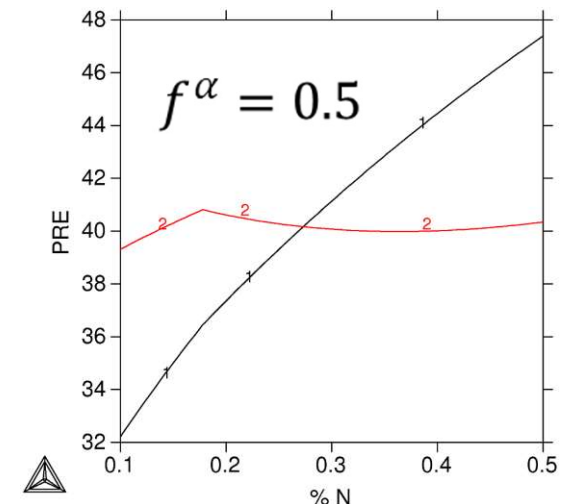
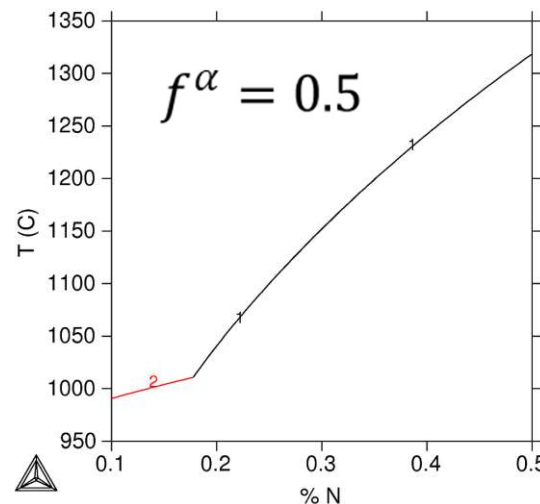


Thermo-Calc Software AB was founded in 1997 and originates in research that had been made at the Royal Institute of Technology (KTH), Stockholm, Sweden.



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.

☐ Software maintenance and support

Thermo-Calc (1984)

DICTRA (1992)

TC-PRISMA (2011)

Software Development Kits



☐ Thermodynamic and Mobility databases

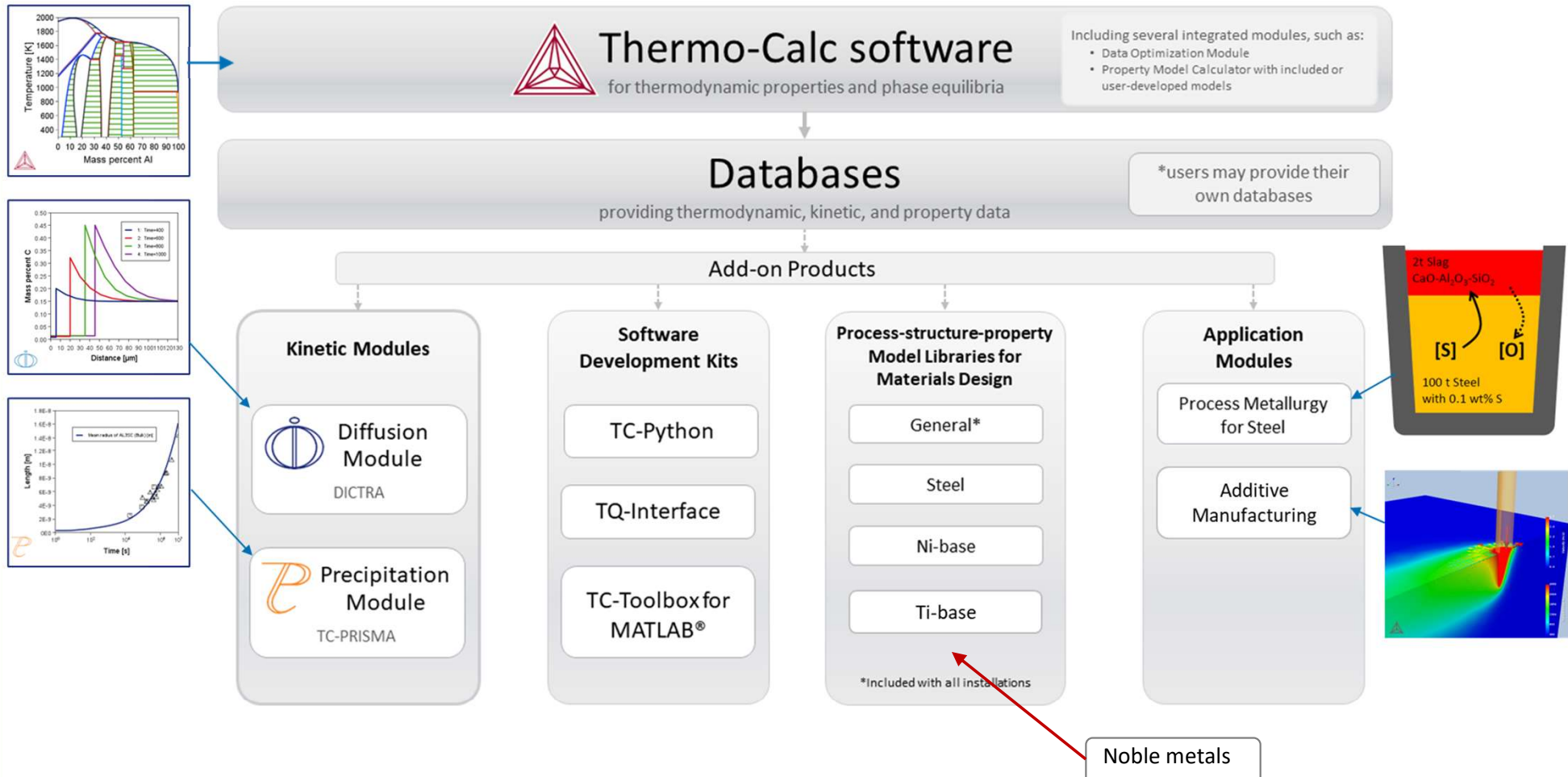


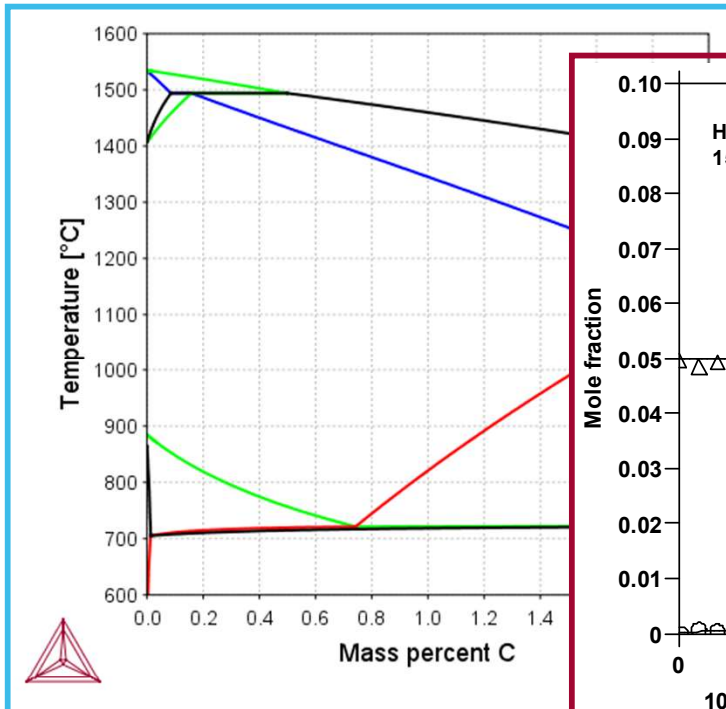
☐ Project work and consulting

☐ Training

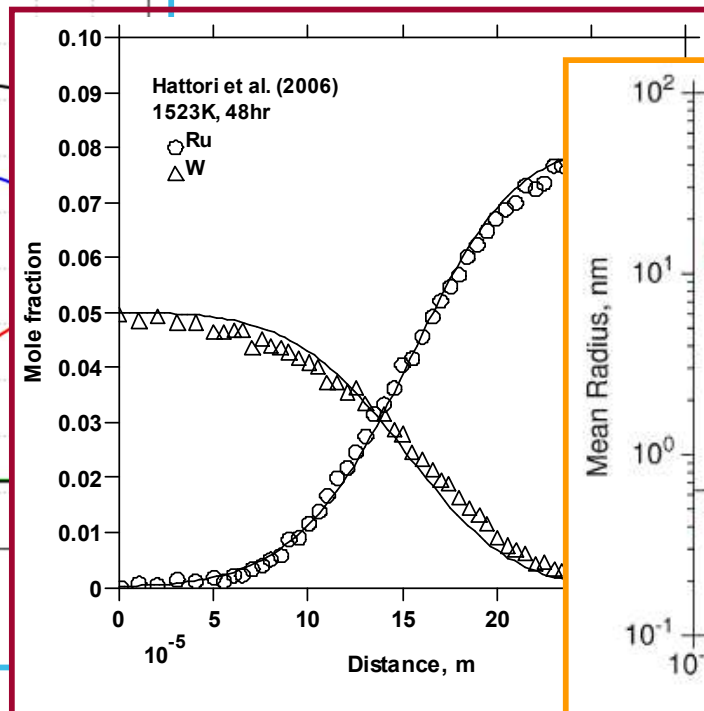


Product overview – TC 2025

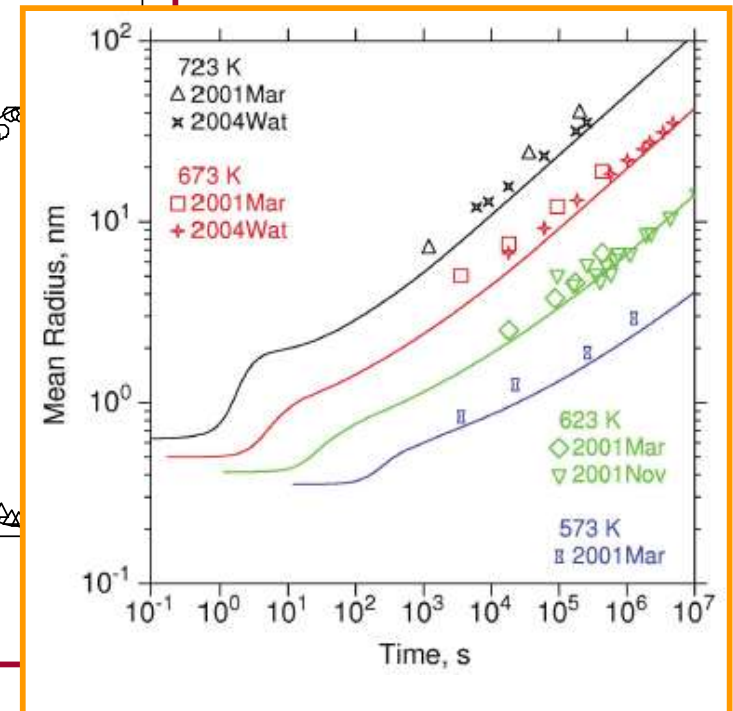




Gibbs energy
= **Phase diagrams**
(equilibrium & metastable
also driving forces!)



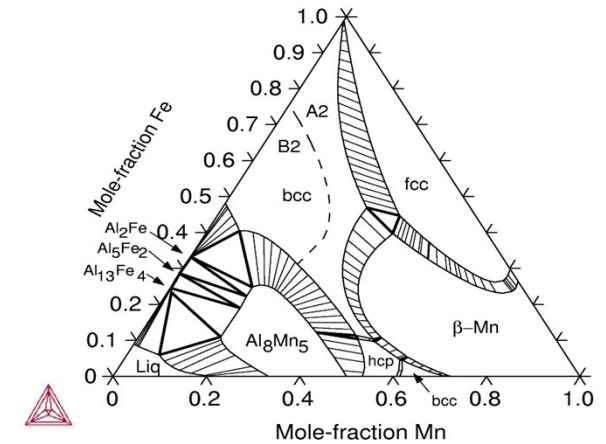
+ Mobility data
= **Diffusion**



+ Interfacial energy
= **Precipitation**

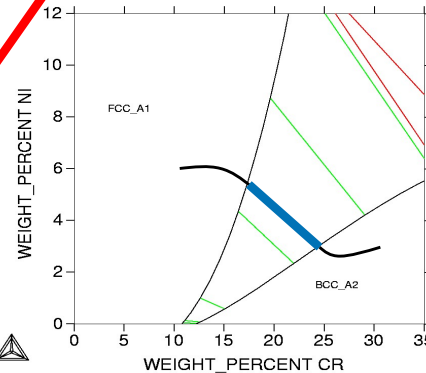


Developing Integrated Codes

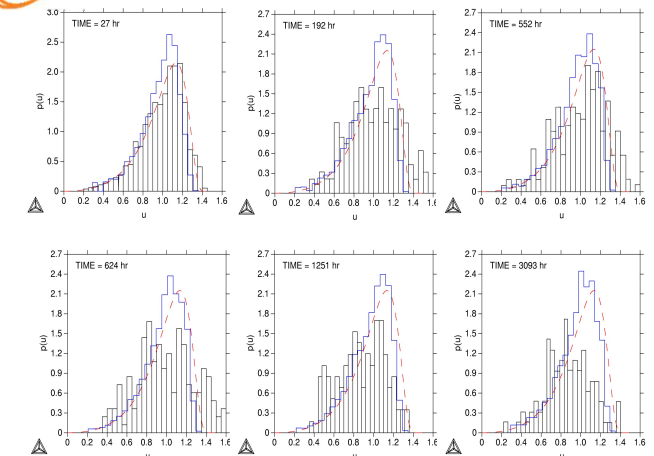
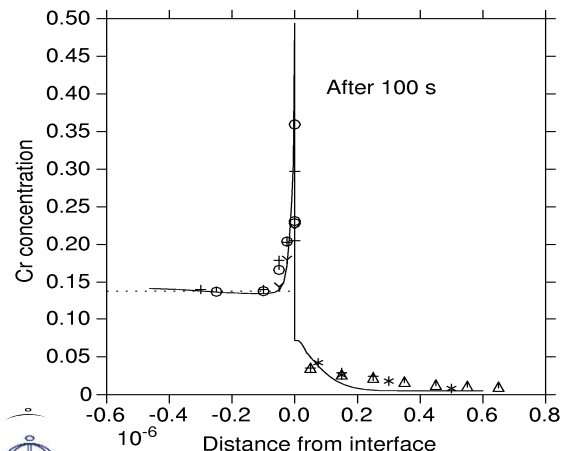


Driving forces

Interfacial energies



Diffusivities



- 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)



Thermo-Calc

Minimization of the total Gibbs free energy under given conditions.

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

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



DICTRA

1-D diffusion simulation –
Numerically solve diffusion equations

Solve Diffusion

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



TC-PRISMA

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

Continuity equation

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

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

Mass balance

What can we calculate, predict, simulate?



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)

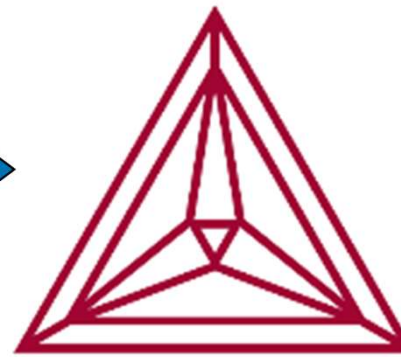


TC-PRISMA

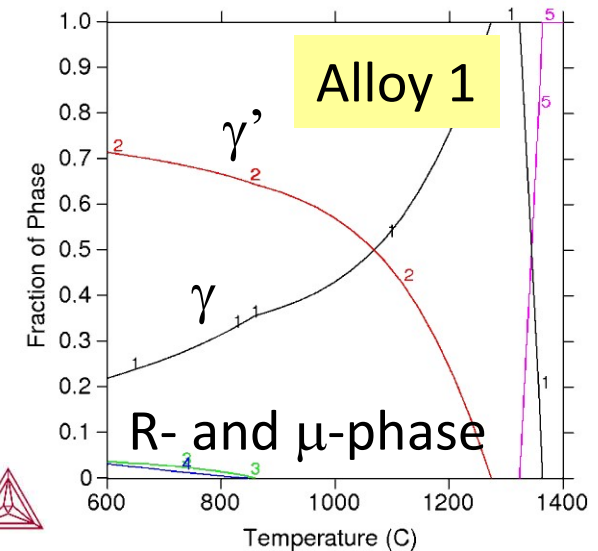
- Particle Size Distribution
- Number Density
- Average Particle Radius
- Volume Fraction
- TTP/CCT
- Average Compositions
- Interface Compositions
- Nucleation Rate
- Critical Radius

Method

Thermodynamic
Database



Thermo-Calc



Description of
Gibbs free energy
for the individual
phases

$$G_m^\phi(T, P, x_i^\phi)$$

Minimization of the
total Gibbs free
energy under given
conditions.

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

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

Result

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....

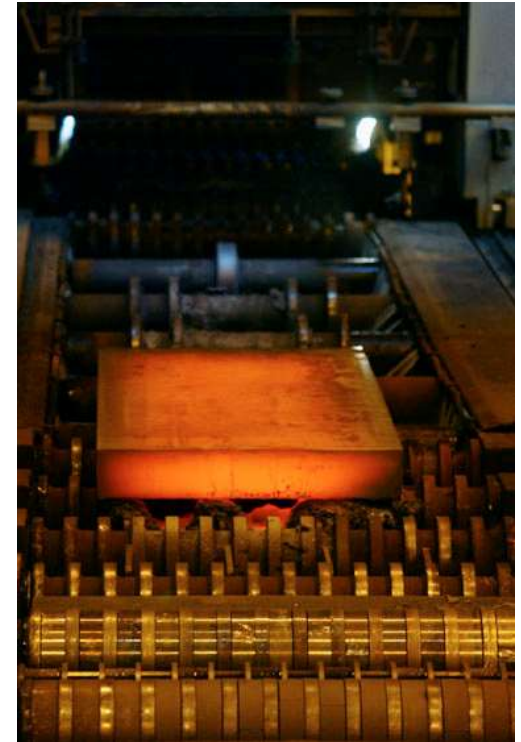


Photo: Stig-Göran Nilsson (2002)

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

Fundamental types of calculations

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

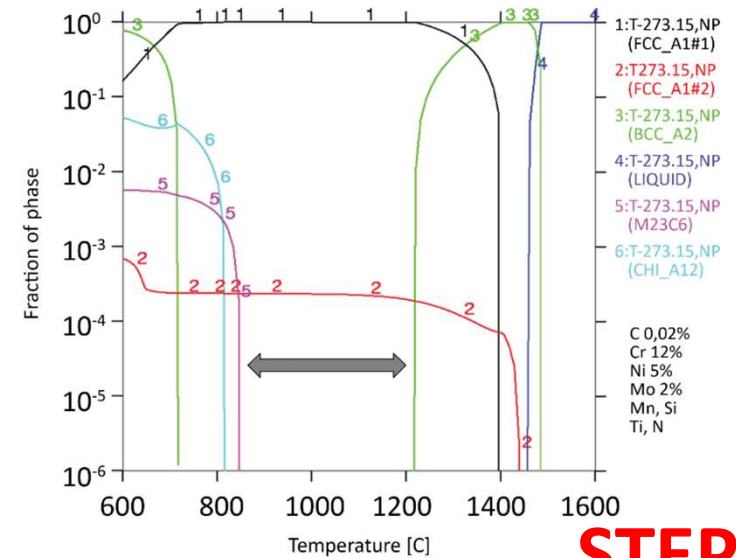
Component	Moles	W-Fraction	Activity	Potential	Ref.State
C	8.6072E-02	2.0000E-02	8.9724E-02	-2.0046E+04	SER
CR	9.9412E-02	1.0000E-01	4.4290E-04	-6.4206E+04	SER
FE	7.7748E-01	8.4000E-01	6.0347E-03	-4.2489E+04	SER
MN	2.8227E-02	3.0000E-02	4.6517E-05	-8.2943E+04	SER
NI	8.8074E-03	1.0000E-02	3.3158E-05	-8.5758E+04	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

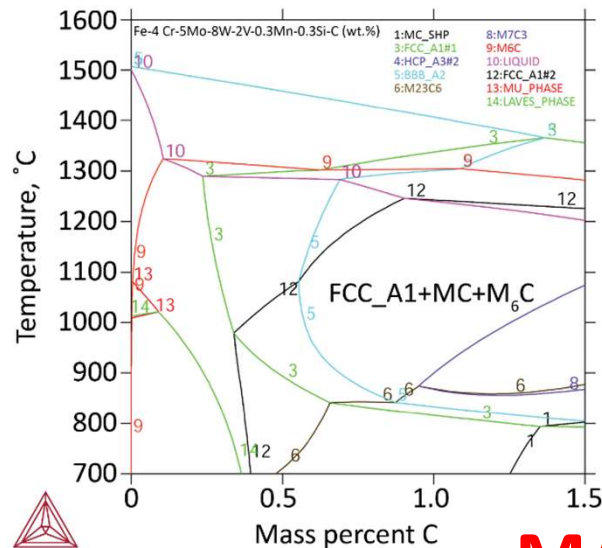
FCC_A1#2 STATUS ENTERED Driving force 0.0000E+00
Number of moles 0.0000E+00, Mass 0.0000E+00
Mass fractions:
FE 9.44835E-01 CR 1.41596E-02 C 3.93605E-03
MN 2.47653E-02 NI 1.23038E-02

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 3.42660E-04
FE 4.00536E-01 MN 5.19435E-02

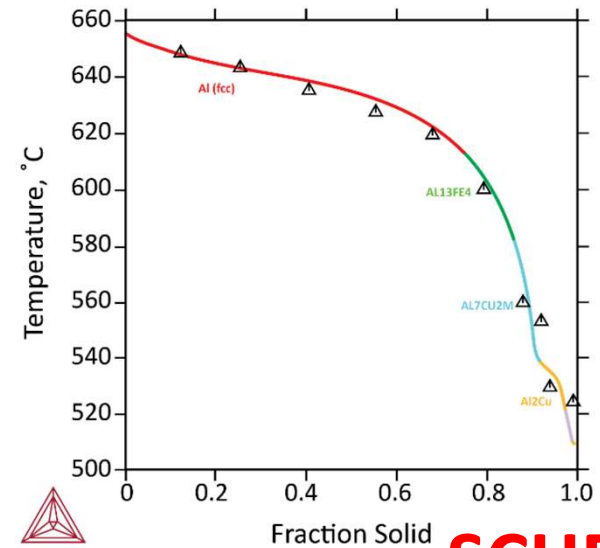
Single Point Equil.



STEP



MAP



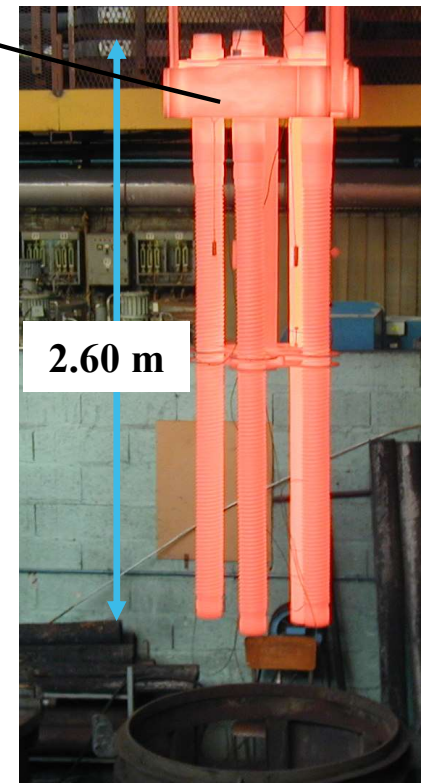
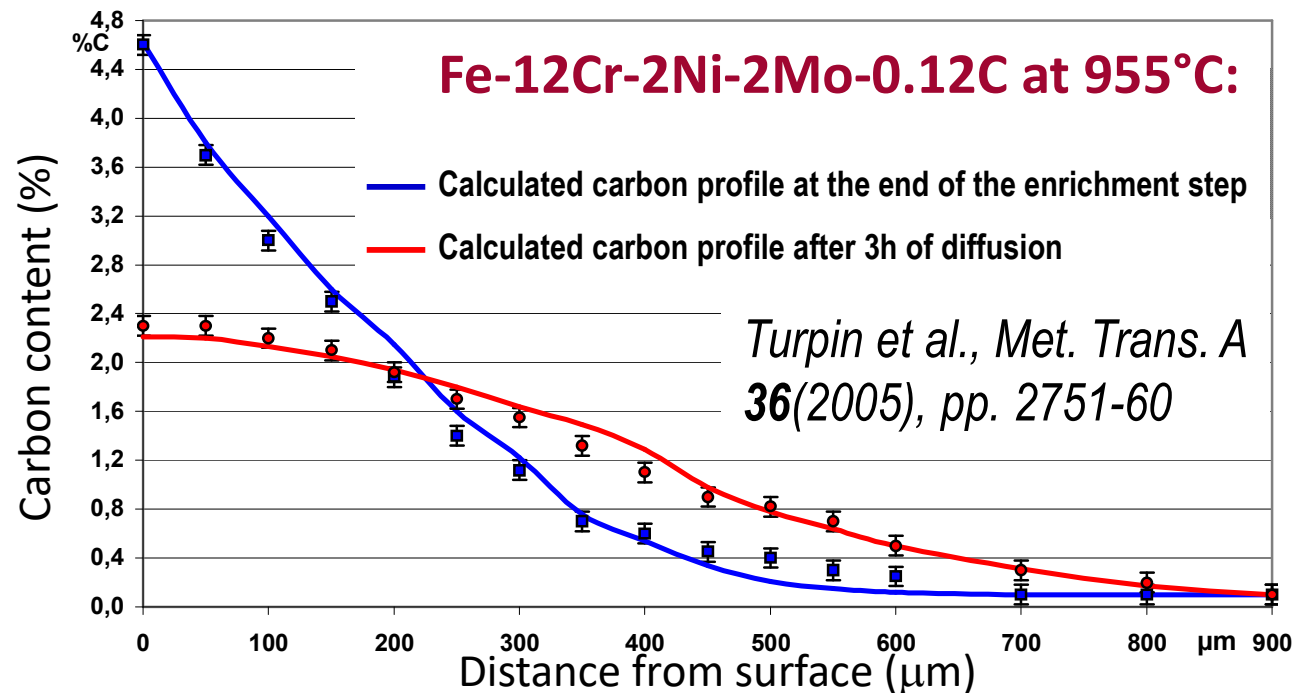
SCHEIL

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...

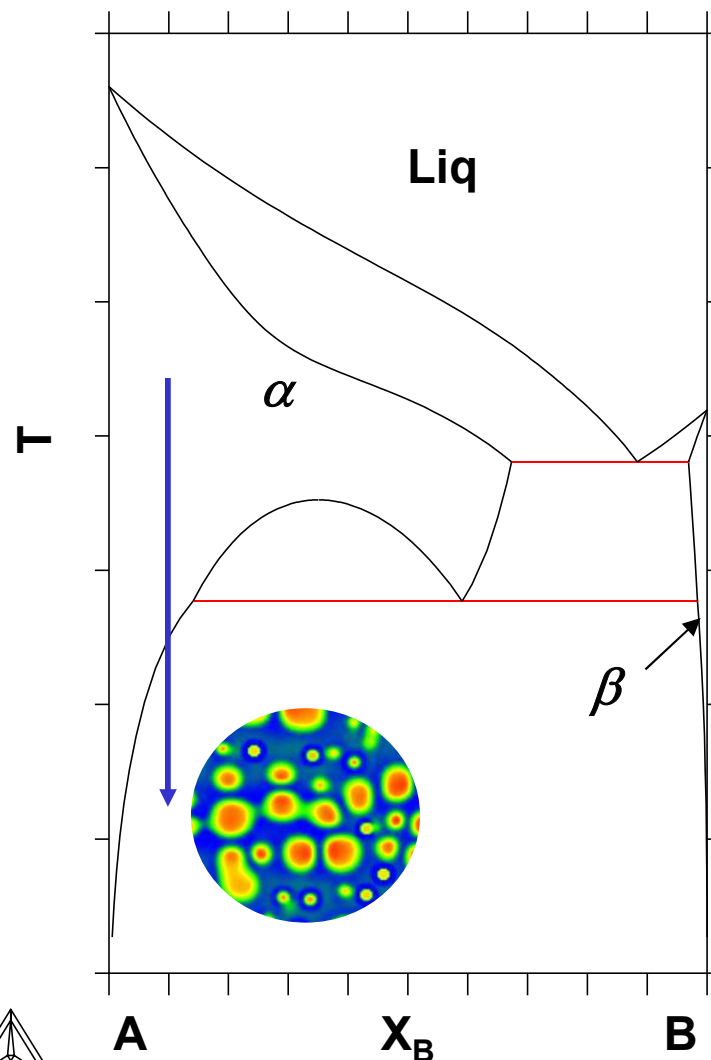


Example: Simulation of carbon evolution in high alloyed steels by Aubert & Duval, France.



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

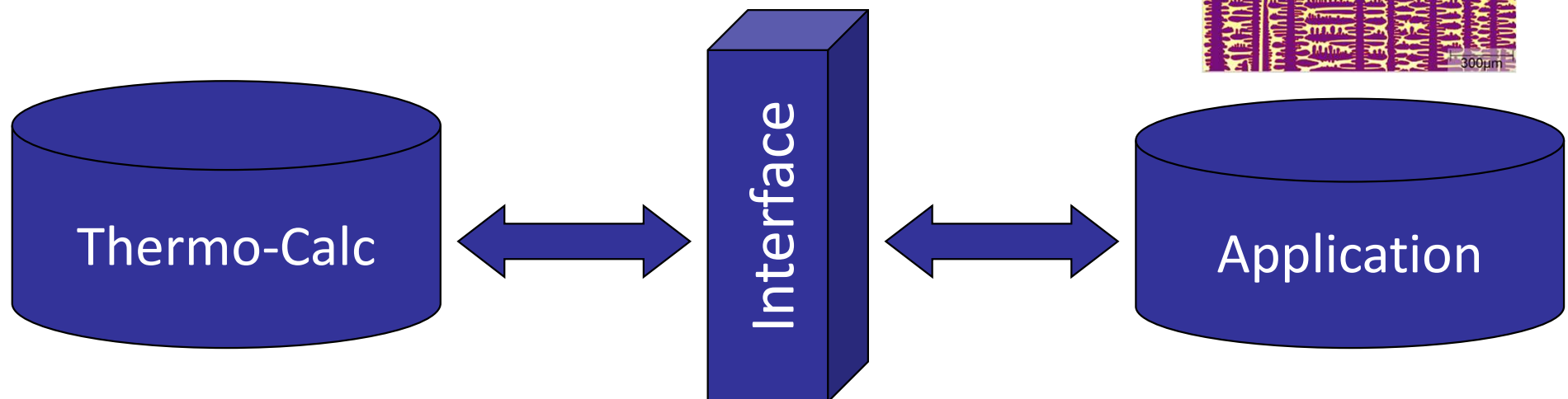
Software Development Kits (SDKs)

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.

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 $\Rightarrow$ All our software tools

- Gibbs free energy, i.e. $G_m^\phi = f(T, P, x_i^\phi)$

☐ Kinetic data $\Rightarrow$ DICTRA, TC-PRISMA, (TC-API's)

- Atomic mobility

☐ Property data

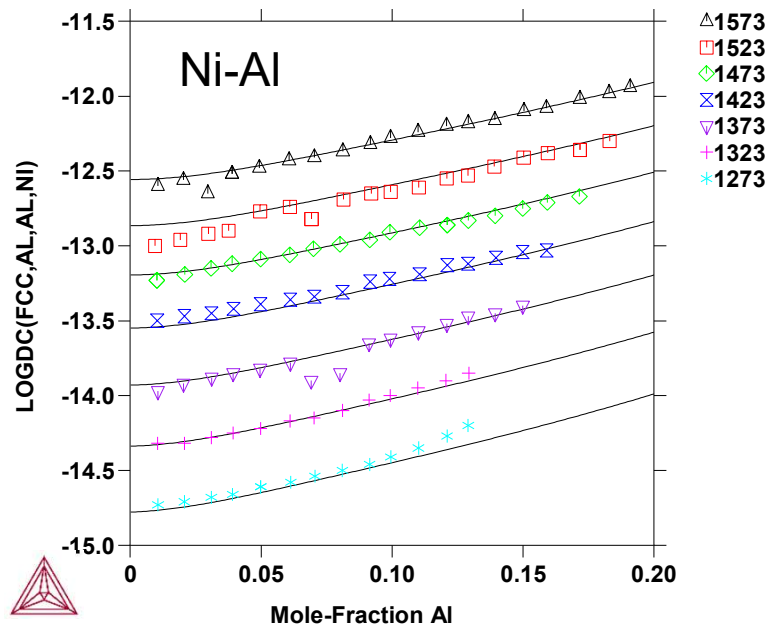
- Molar volume	$\Rightarrow$ TC, TC-PRISMA
- Thermal conductivity/resistivity/diffusivity	$\Rightarrow$ TC
- Electric resistivity/conductivity	$\Rightarrow$ TC
- Liquid viscosity/surface tension	$\Rightarrow$ TC
- <i>Interfacial energies (not in database)</i>	$\Rightarrow$ TC-PRISMA

A wide range of thermodynamic databases are available for:

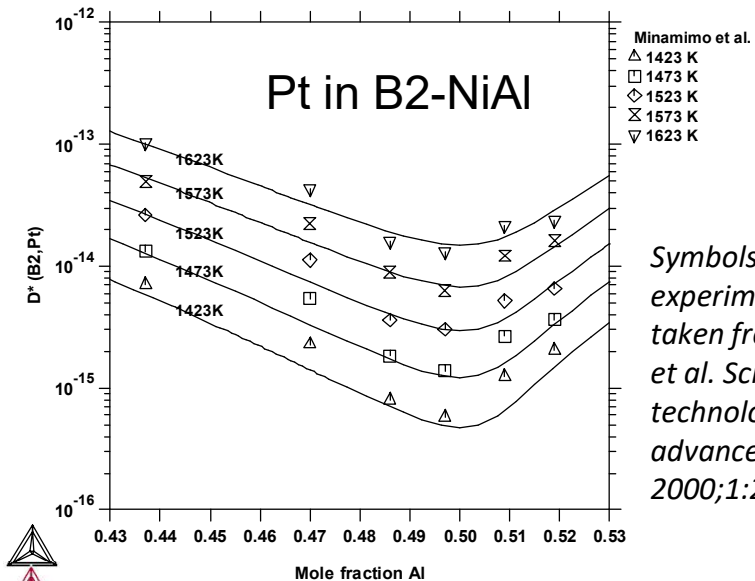
- ☐ Steels and Fe-alloys
- ☐ Nickel-base superalloys
- ☐ Al-/Ti-/TiAl-/Mg-/Cu-/Zr/Mo-/Nb-alloys
- ☐ High Entropy alloys (HEA)
- ☐ Noble metal alloys, Solder alloys
- ☐ Electronic materials, magnetic materials, ultra-pure Si-alloys
- ☐ Gases, pure inorganic/organic substances and general alloys
- ☐ Slag, 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

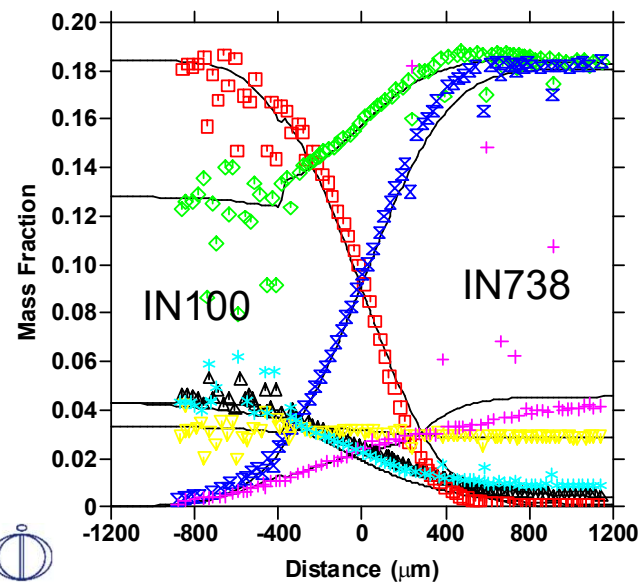
- | | |
|--|--|
| ☐ Steels and Fe-alloys | ☐ Mg alloys |
| ☐ Nickel-base superalloys | ☐ Solder alloys |
| ☐ Aluminium alloys | ☐ Si |
| ☐ Noble metal alloys | ☐ Mo alloys |
| ☐ High Entropy alloys | ☐ Nb alloys |
| ☐ Ti alloys | ☐ Zr alloys |
| ☐ Cu alloys | |



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.

□ 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

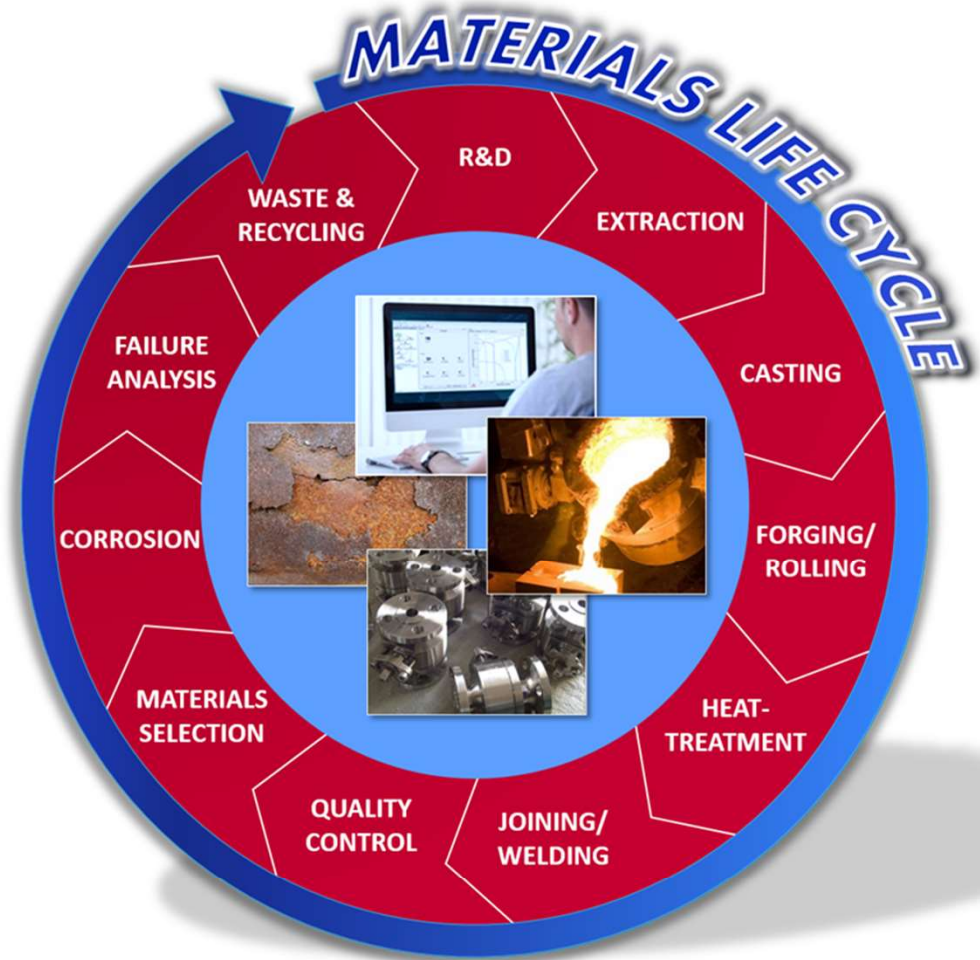


□ Academia (*material science, mech. engineering, metallurgy....*)



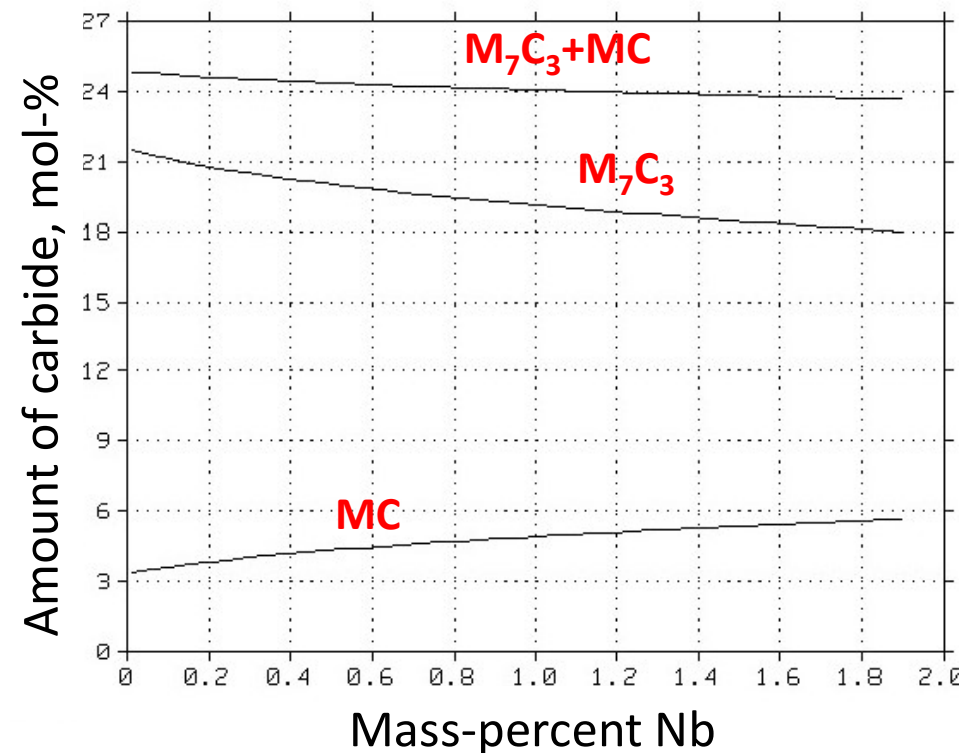
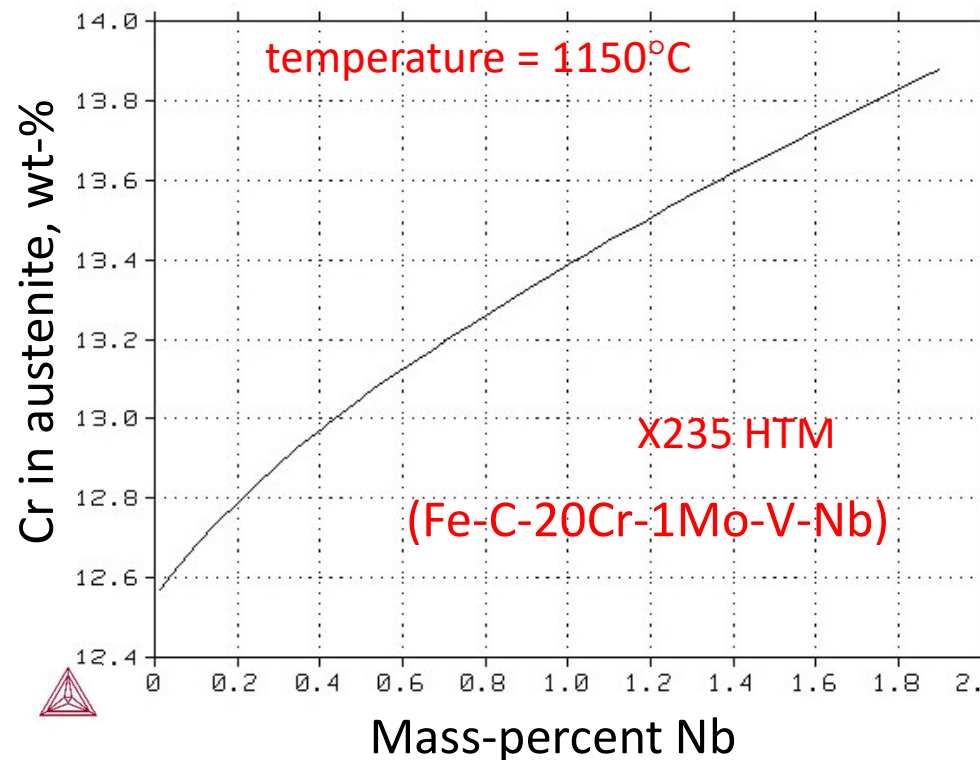
Examples with application to the materials life cycle

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.



Ascertaining the Influence of Alloying Elements

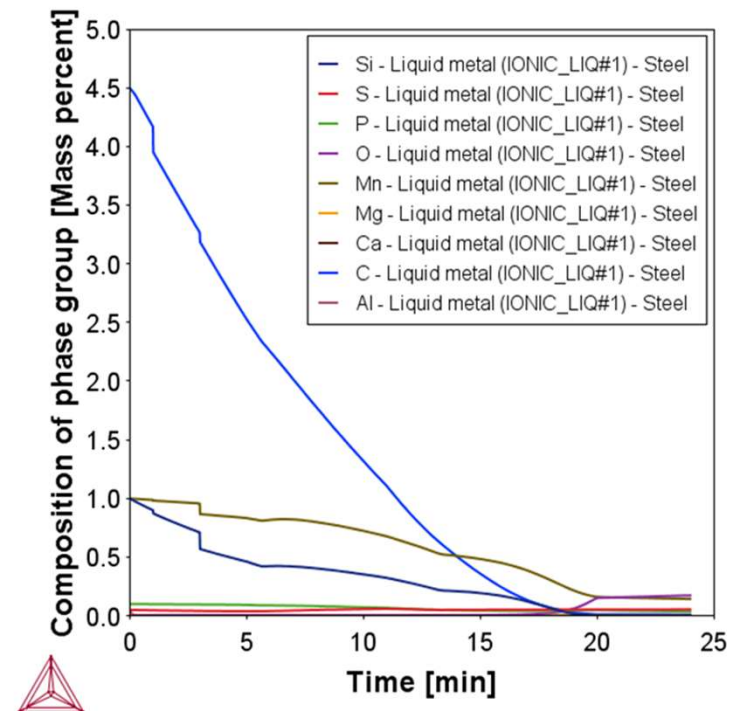
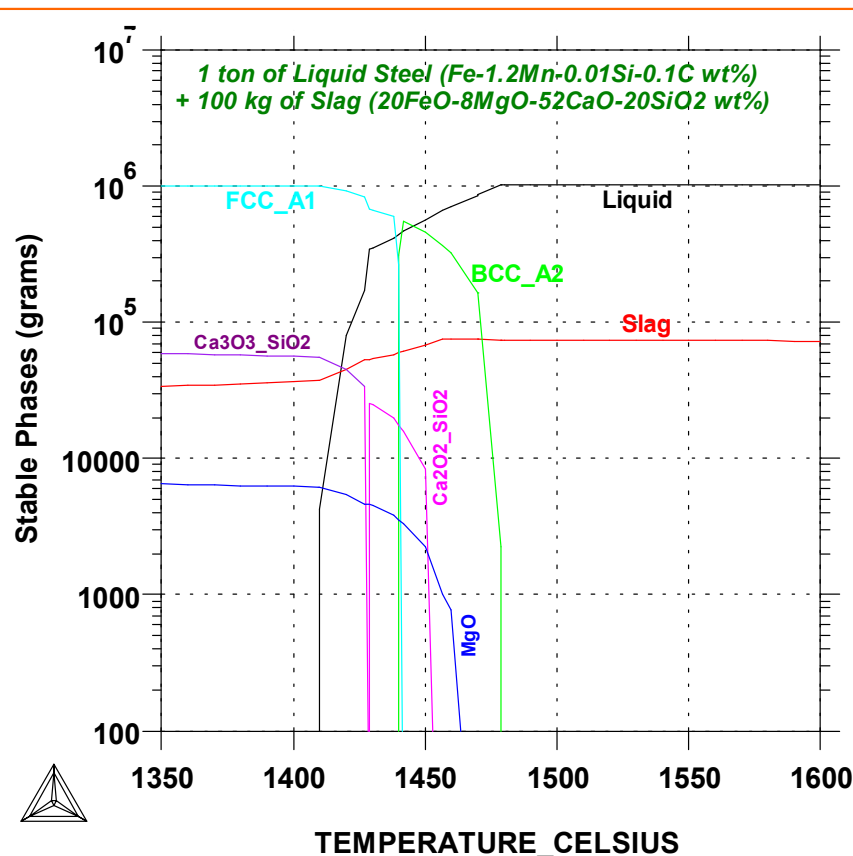
Example: Influence on Chromium solubility when replacing V with Nb



V + Nb = constant = 5.27 at. %

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/solidification

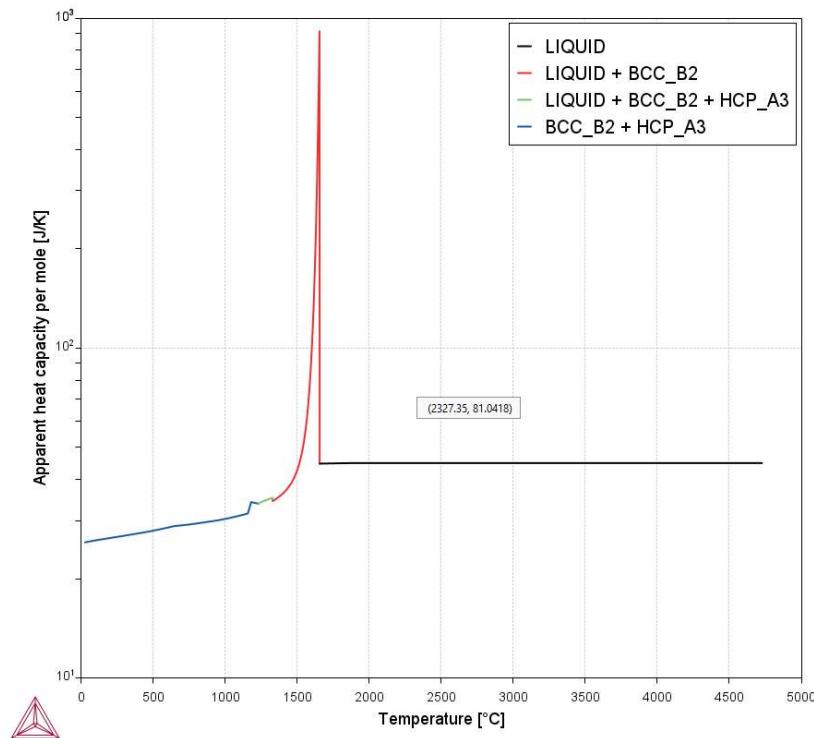
Thermo-Calc can be used to generate data to input into FEM codes for casting or AM.

- ☐ Solidus/liquidus temperatures
- ☐ Fraction solid curve
- ☐ Heat capacity
- ☐ Enthalpy
- ☐ Thermal expansion
- ☐ Thermal conductivity
- ☐ Density / Molar volume
- ☐ Viscosity
- ☐ Surface tension
- ☐ Driving force for evaporation

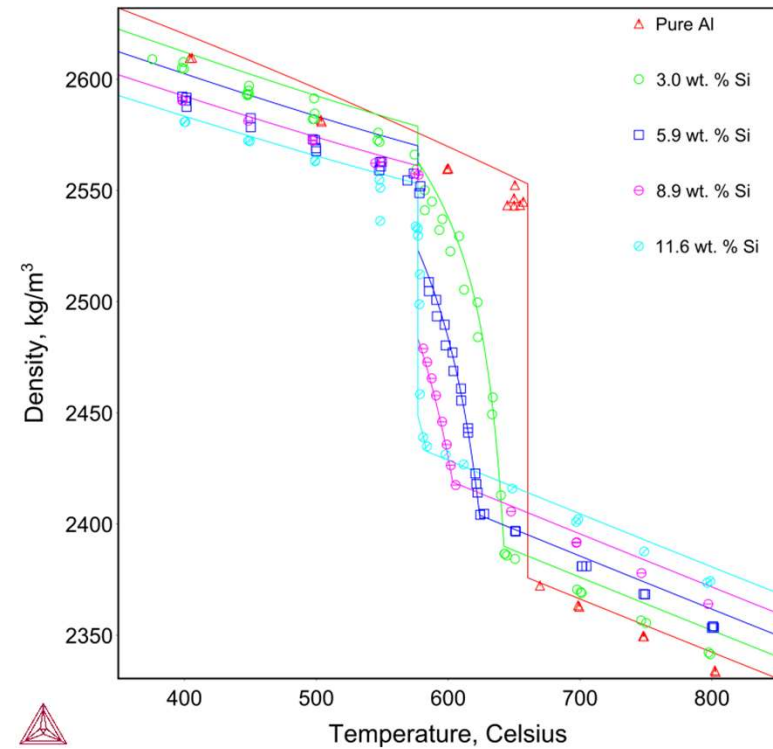


These quantities can of course also be used inside Thermo-Calc itself.

Example results



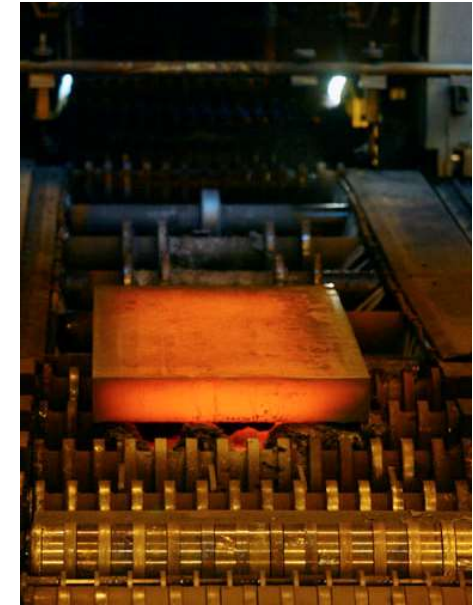
Extended Scheil calculation, showing apparent heat capacity as function of T, to be used in the AM module.



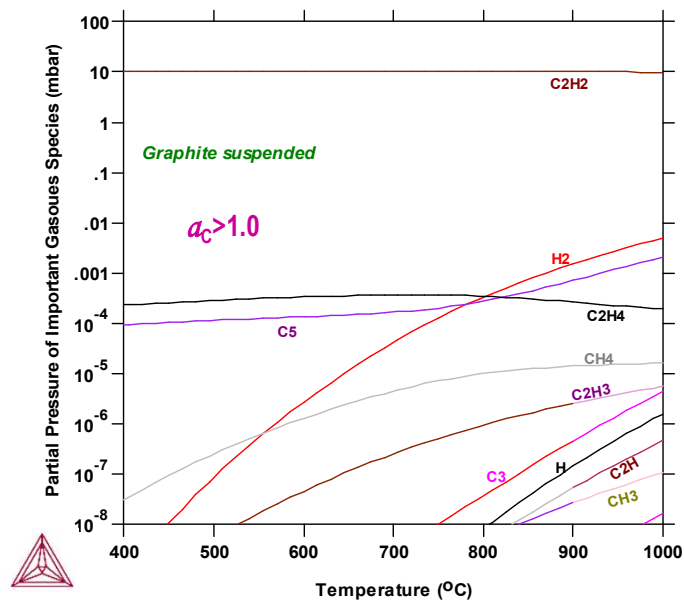
The effect of Si content on the density of Al-Si alloys

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

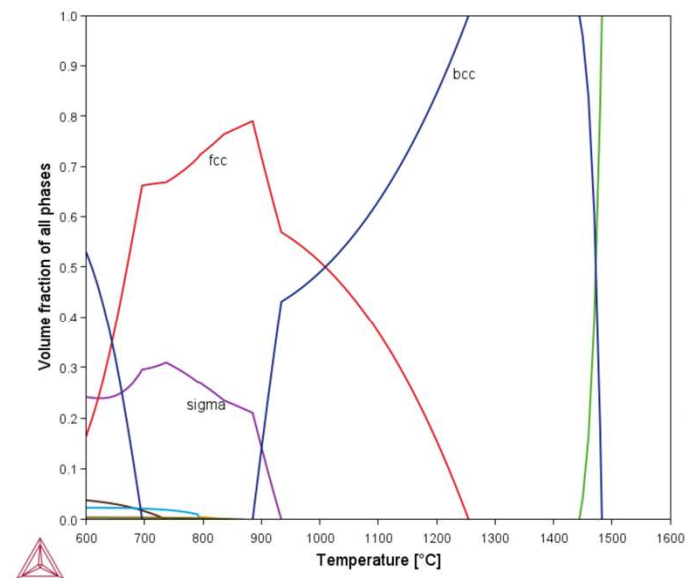
- ❑ Equilibrium between alloy and gas phase as a function of temperature and composition
- ❑ Predict formation of phases / volume-fractions etc.
- ❑ Gas phase reactions, gas speciation
- ❑ Oxide scale formation



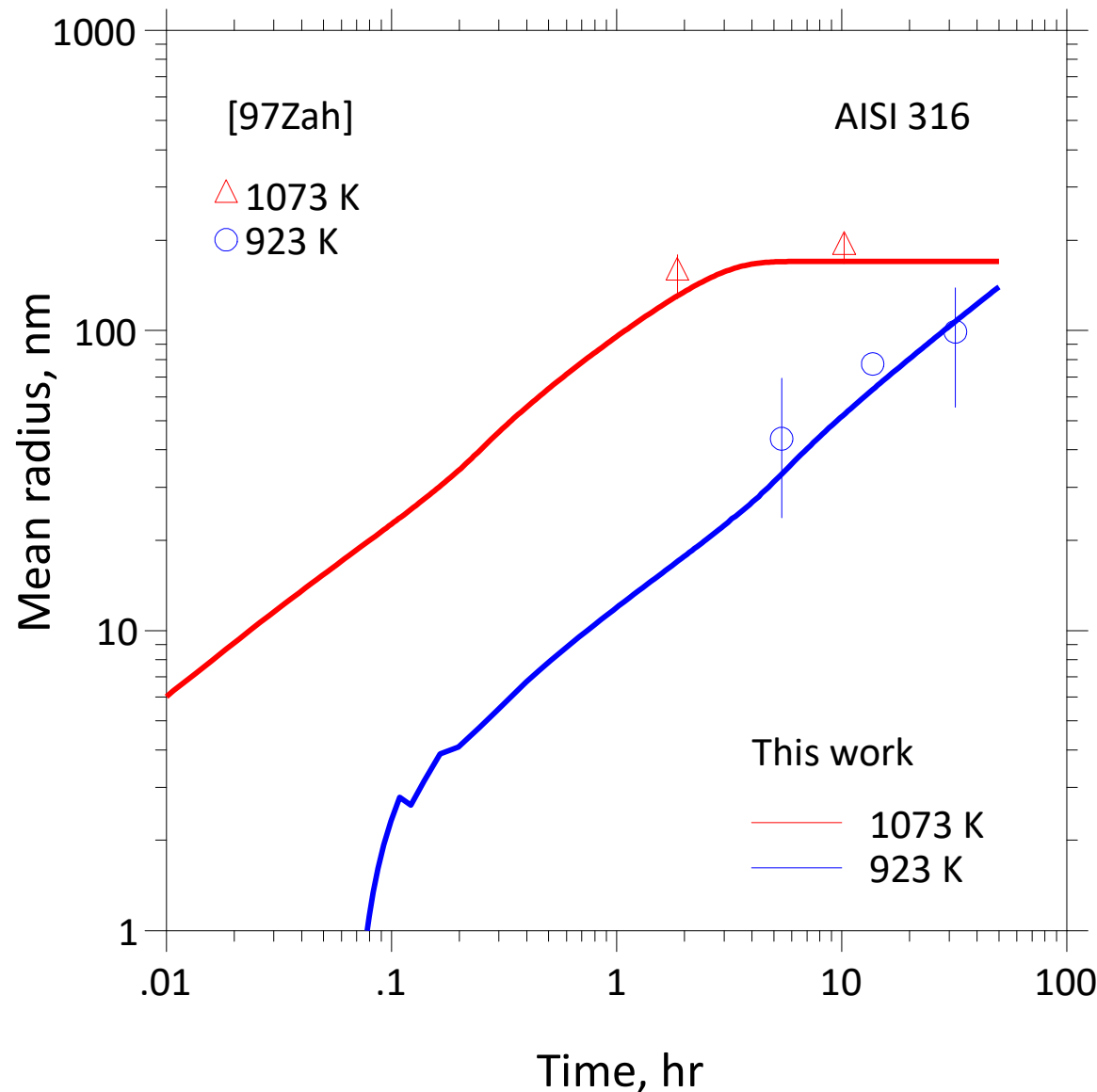
Decomposition of Acetylene at 10 mbar



Phases in stainless steel



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

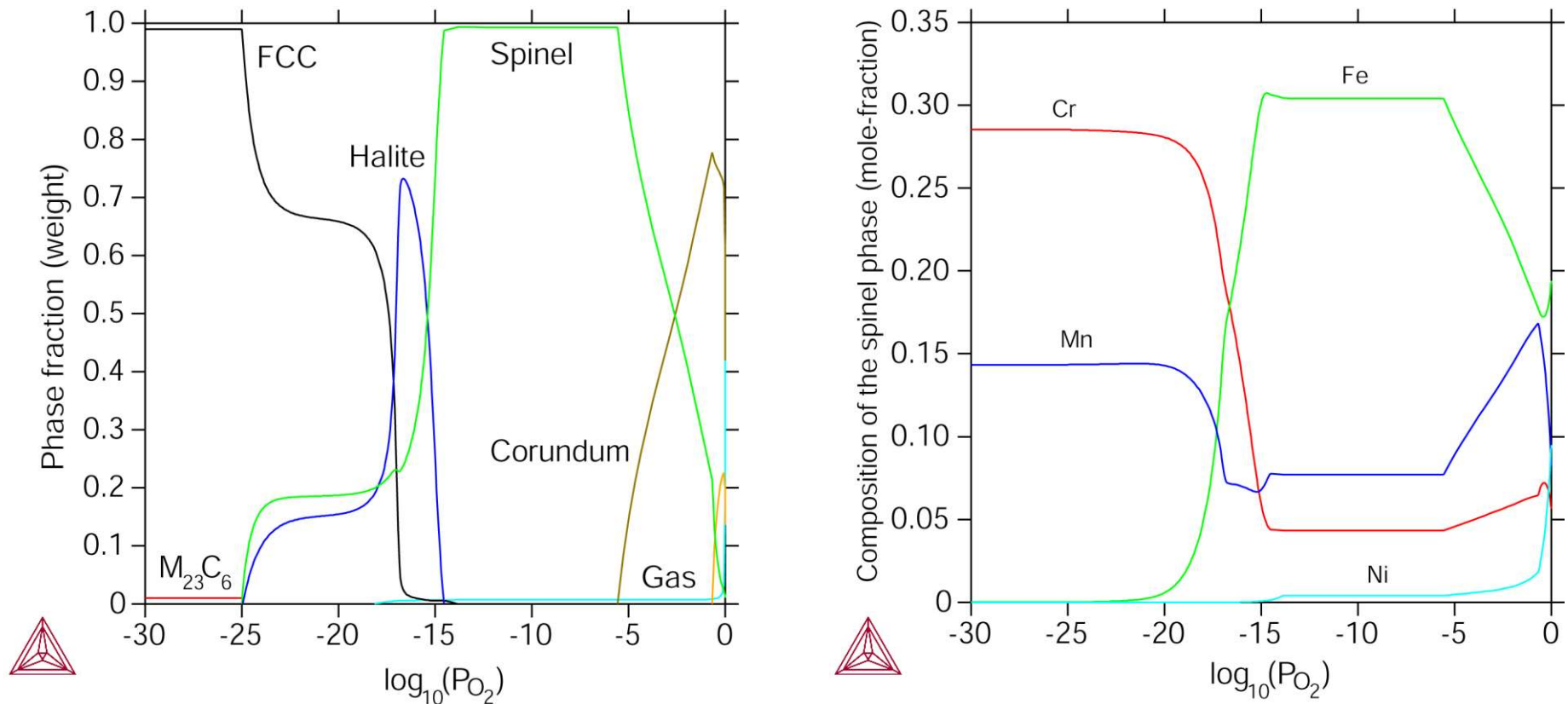
$\sigma = 0.3 \text{ J/m}^2$

800 °C

γ -grain size = 1000 μm

$\sigma = 0.2 \text{ J/m}^2$

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



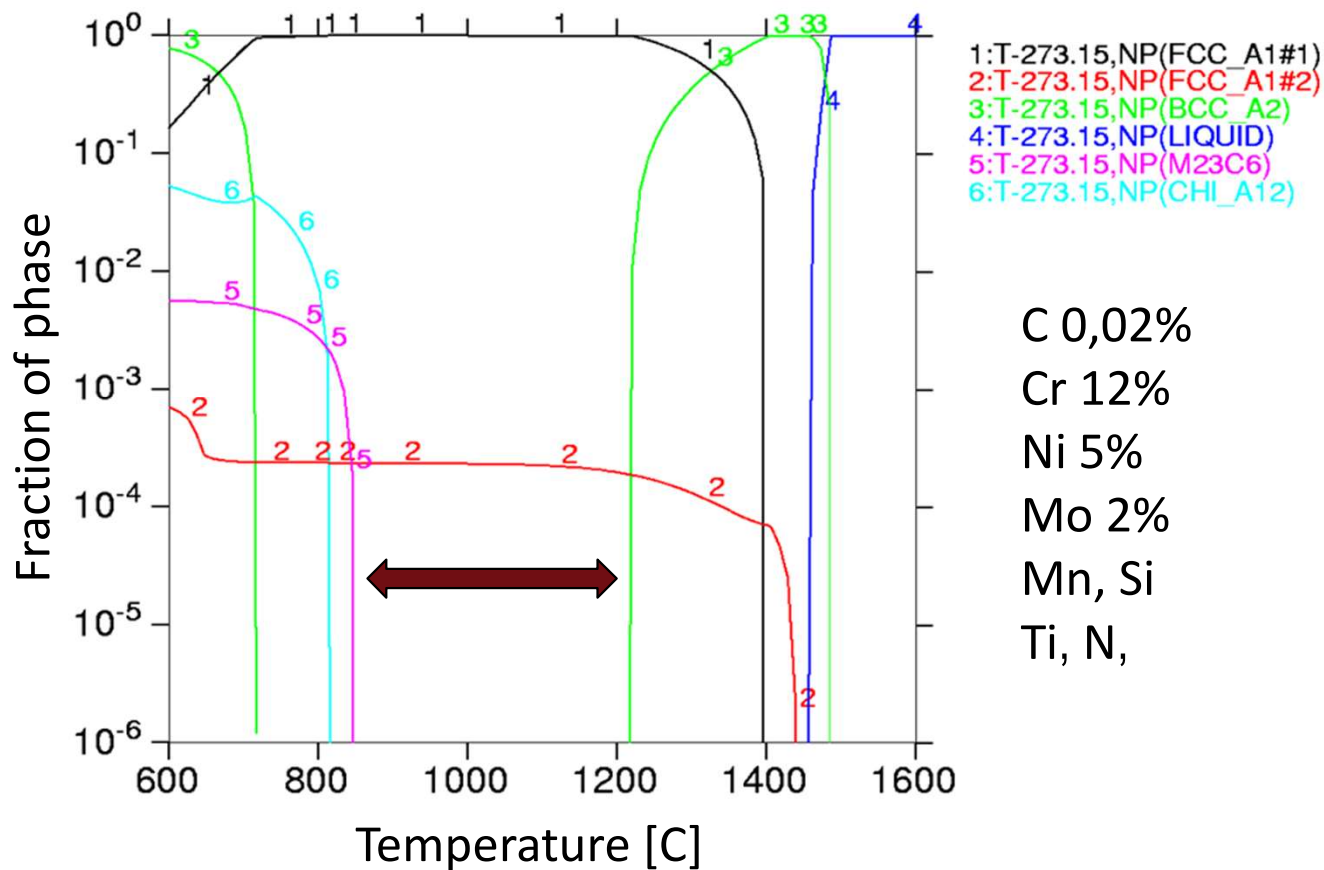
Below the outer scale (rich in corundum) an Fe-Mn rich spinel is formed and next to the substrate a layer with halite and a Cr-Mn rich spinel, which is verified experimentally in the work by Douglas et al [1].

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

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

Selecting optimum temperature for operation

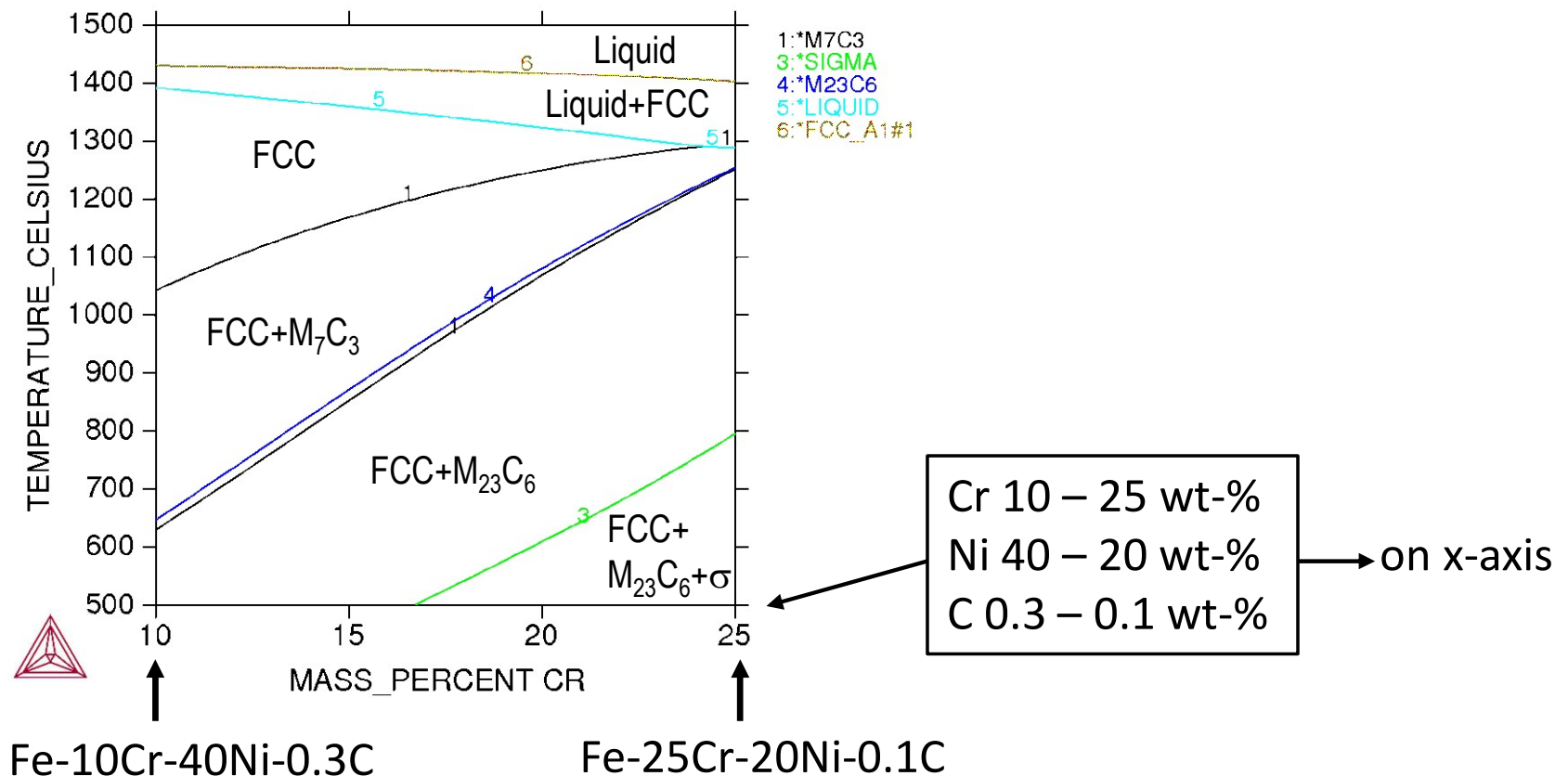
Safe forging of super-martensitic stainless in γ -field

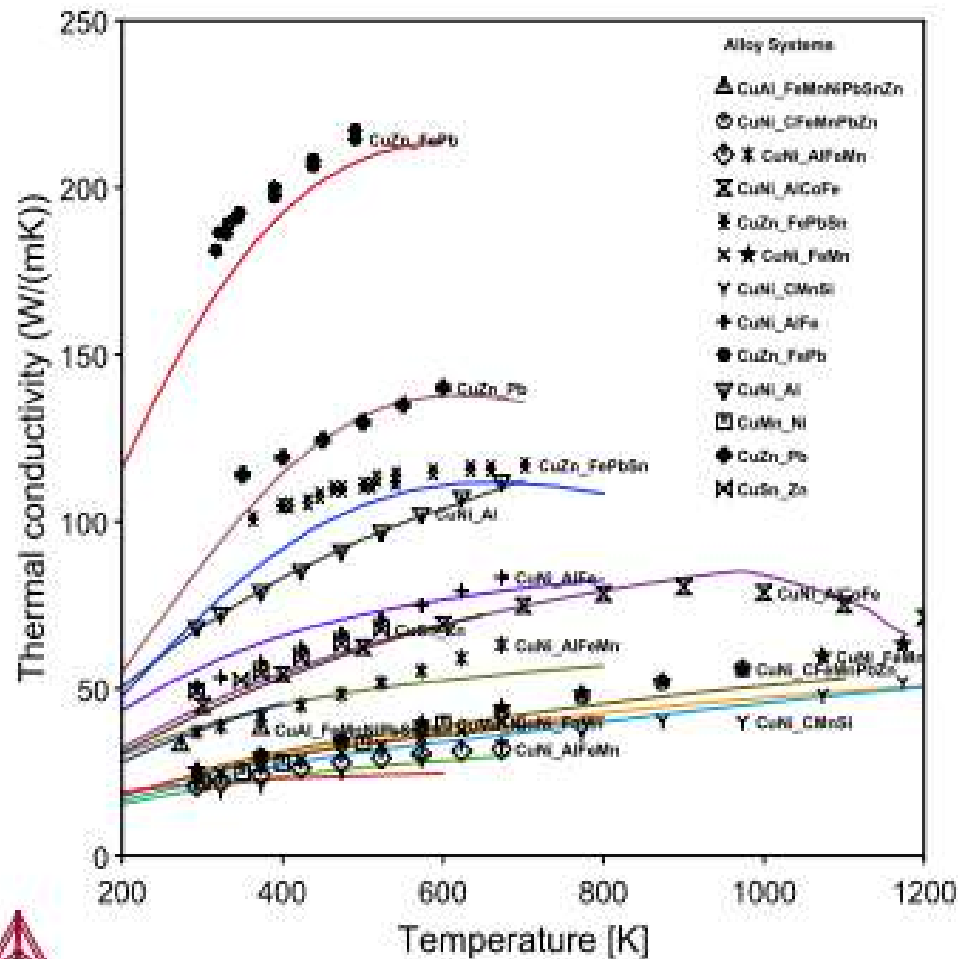


Courtesy André Costa e Silva

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





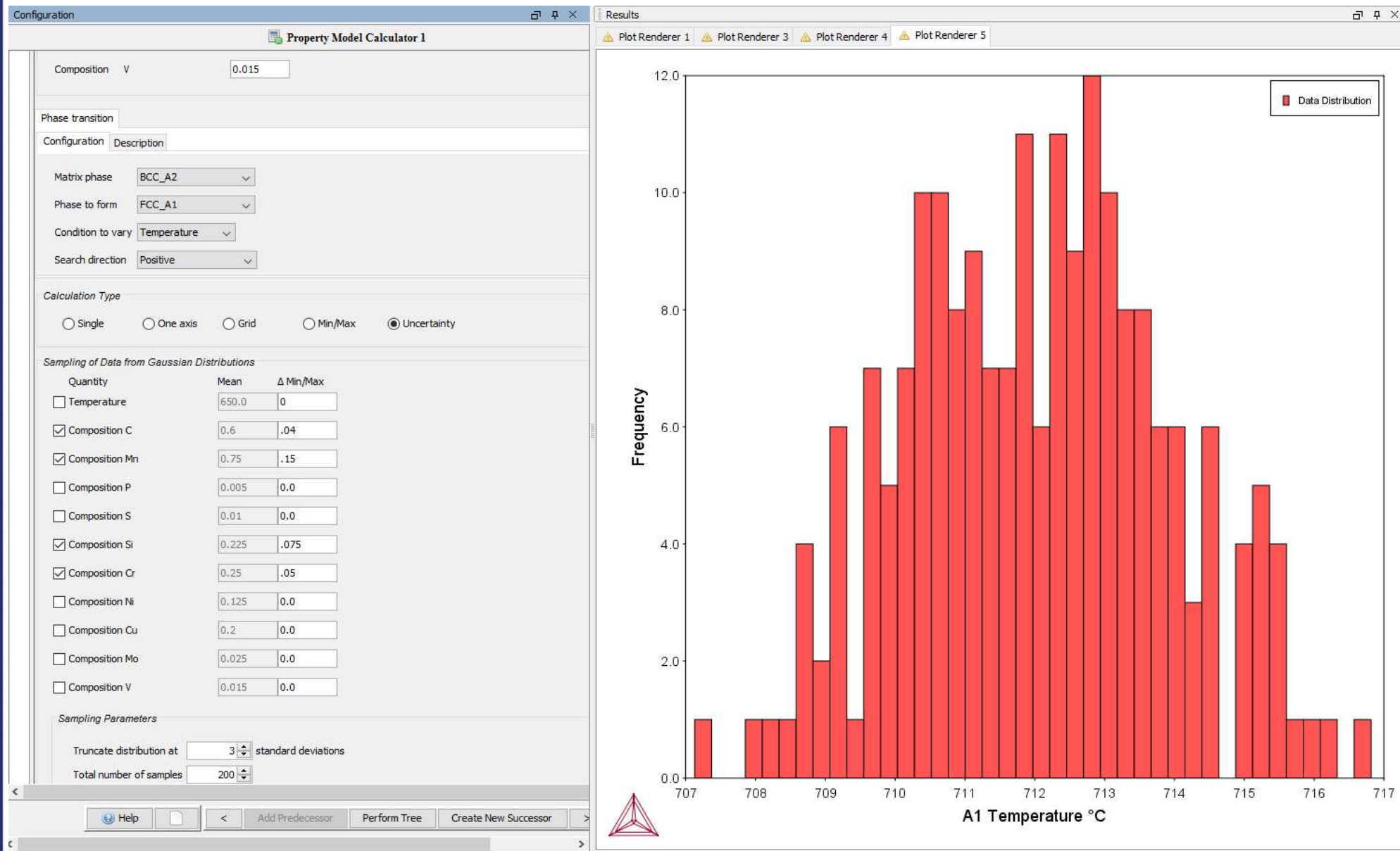
Various thermo-physical properties can be important when selecting material.

This diagram shows the Thermal conductivity versus temperature for various Cu-based alloys.

Notation: *CuNi_AlFeMn* indicates a Cu-alloy with Ni as the major alloying element and Al, Fe, Mn as minor alloying elements.

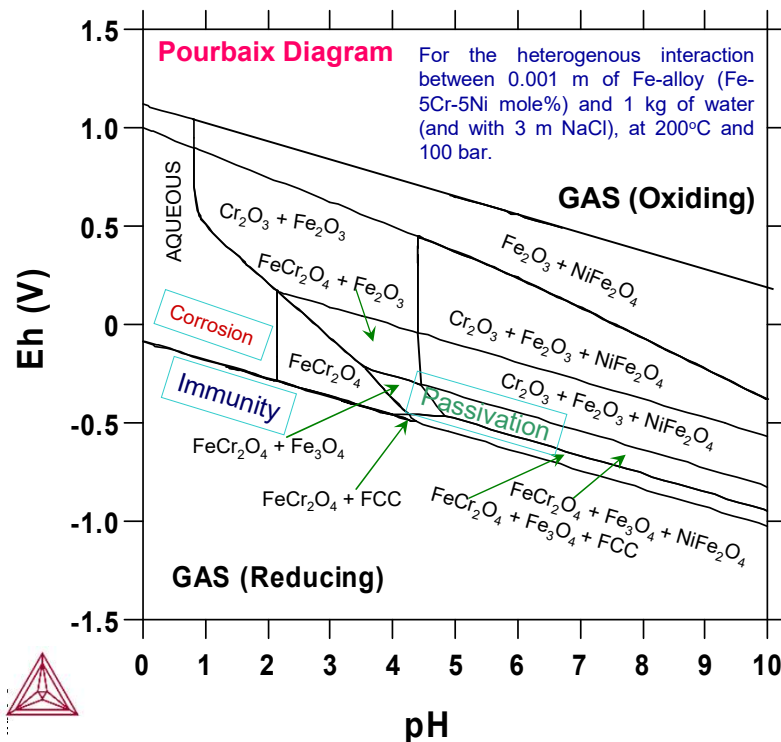
Calculations were made using the “Equilibrium with Freeze-in Temperature” model with TCCU6.0

Uncertainty / Sensitivity analysis



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: $\gamma + \gamma'$ in Ni Superalloy
CMSX-2 at 850°C.

Some definitions

- 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.

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.

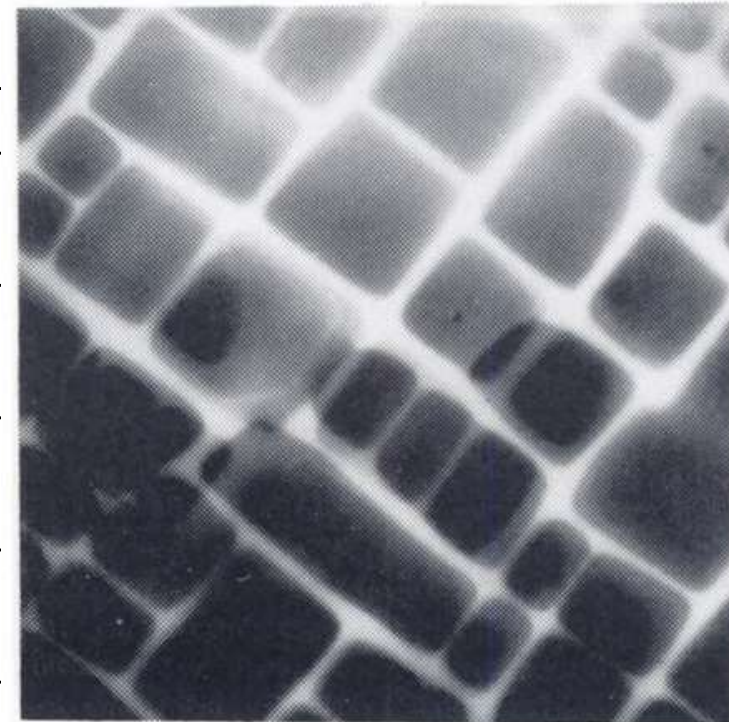
Example: Calculate the liquidus temperature of a metallic alloy.
Set the liquid as **fixed** to 1 mole (if the system size is 1 mole)

Single Equilibrium, Example 2

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 **atomic-%**

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
(ordered phase)?

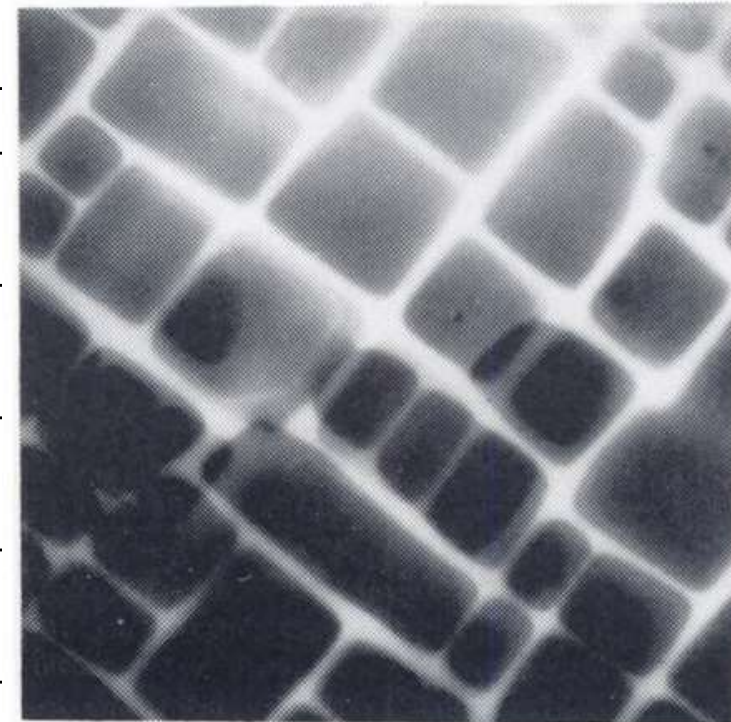
Blavette, D. et al. "AN ATOM-PROBE STUDY OF SOME FINE-SCALE MICROSTRUCTURAL FEATURES IN Ni-BASED SINGLE CRYSTAL SUPERALLOYS." *Superalloys*, 1988 305-314.

Single Equilibrium, Example 2

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?

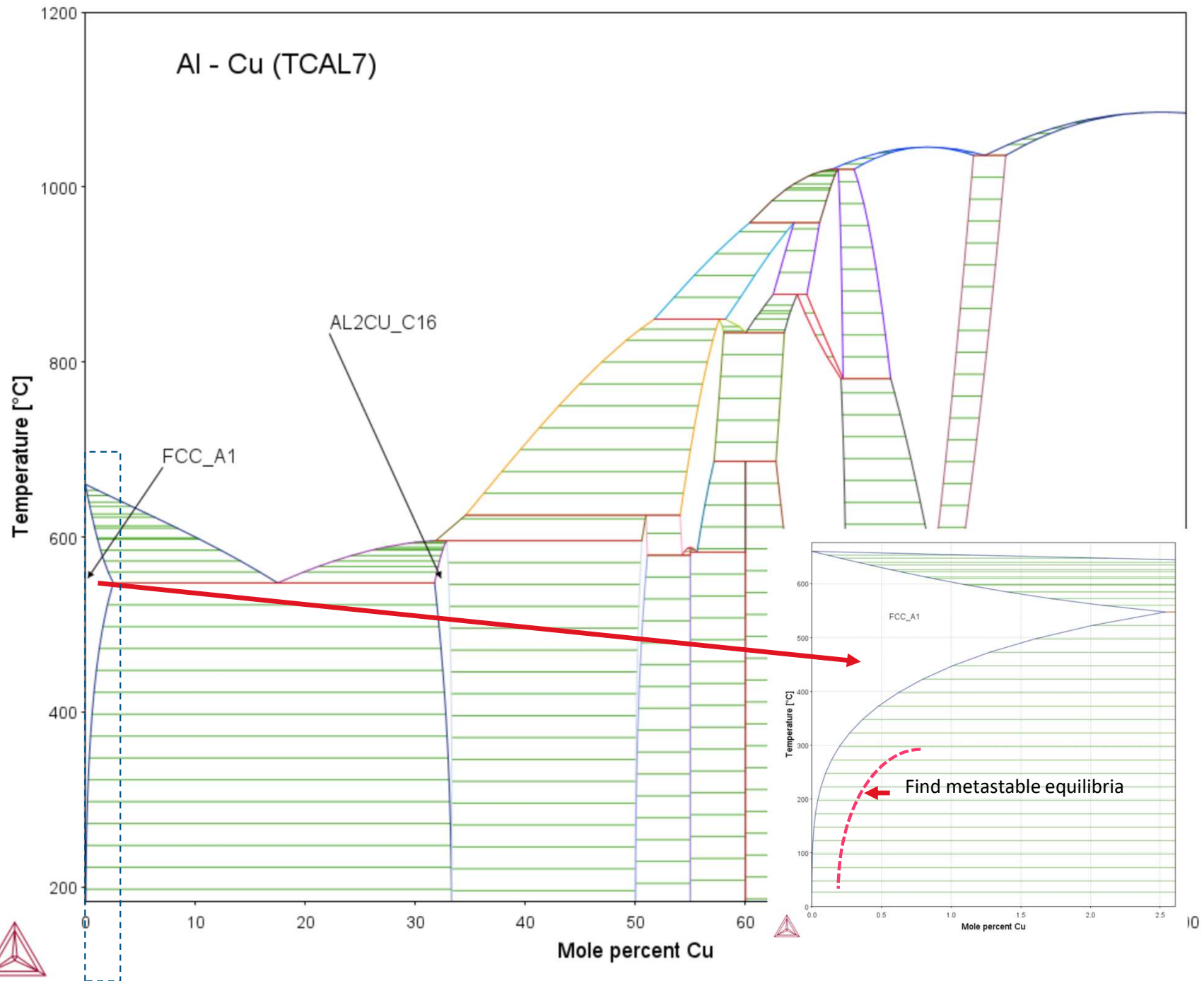
-- the second in the table, $x(\text{Ni})=0.706$ (close to 0.75, Ni_3Al)

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

Questions & Answers

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

Single Equilibrium, Example 3



Single Equilibrium, Example 3

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.

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.

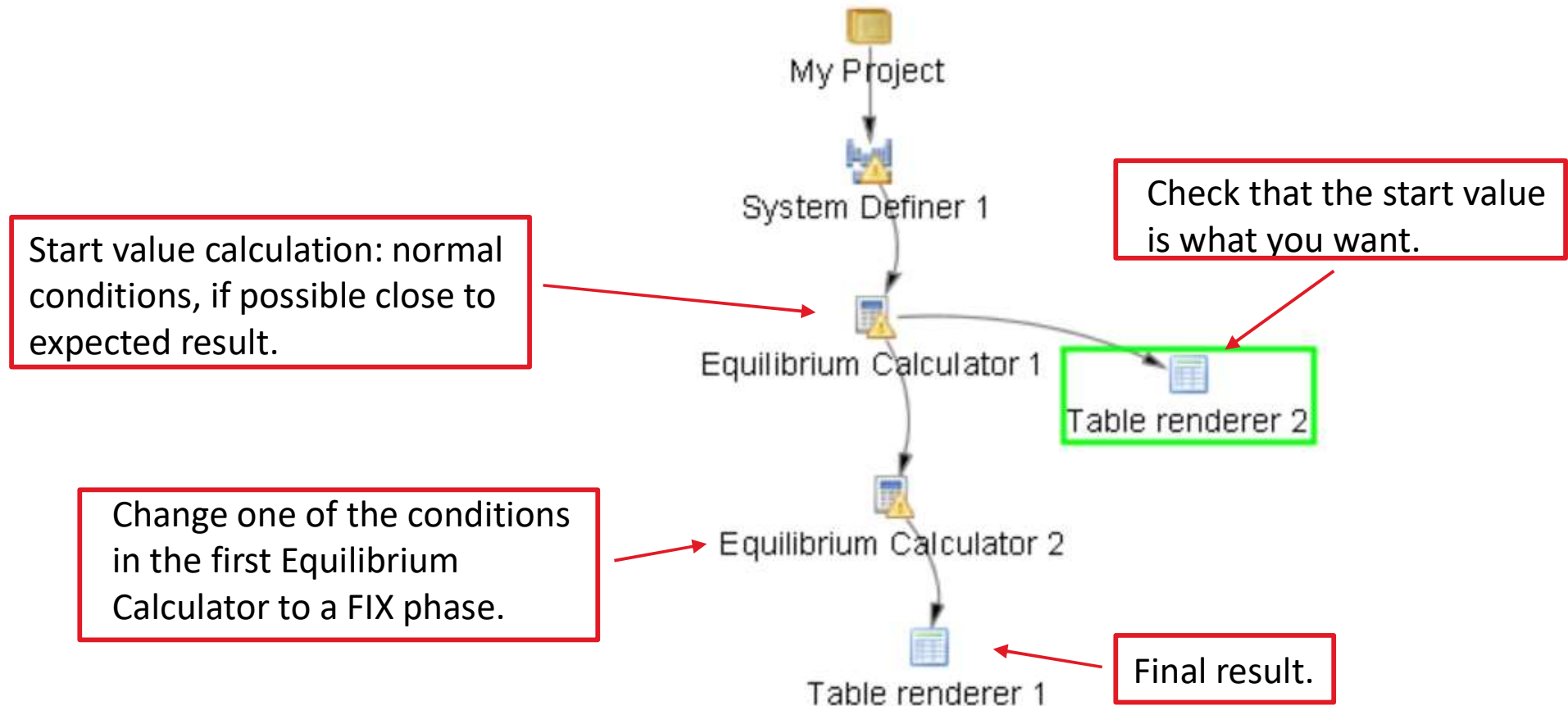
Setting a phase fix takes up one degree of freedom, i.e. it is equal to setting a condition. The fix condition is often a more difficult condition to find the equilibrium for than just using conditions on the standard state variables, T , N , $W(..)$ etc. It can be very dependent on start values.

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

Project



Single Equilibrium, Example 3

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)



What is the most suitable database?

Should I suspend any phases?

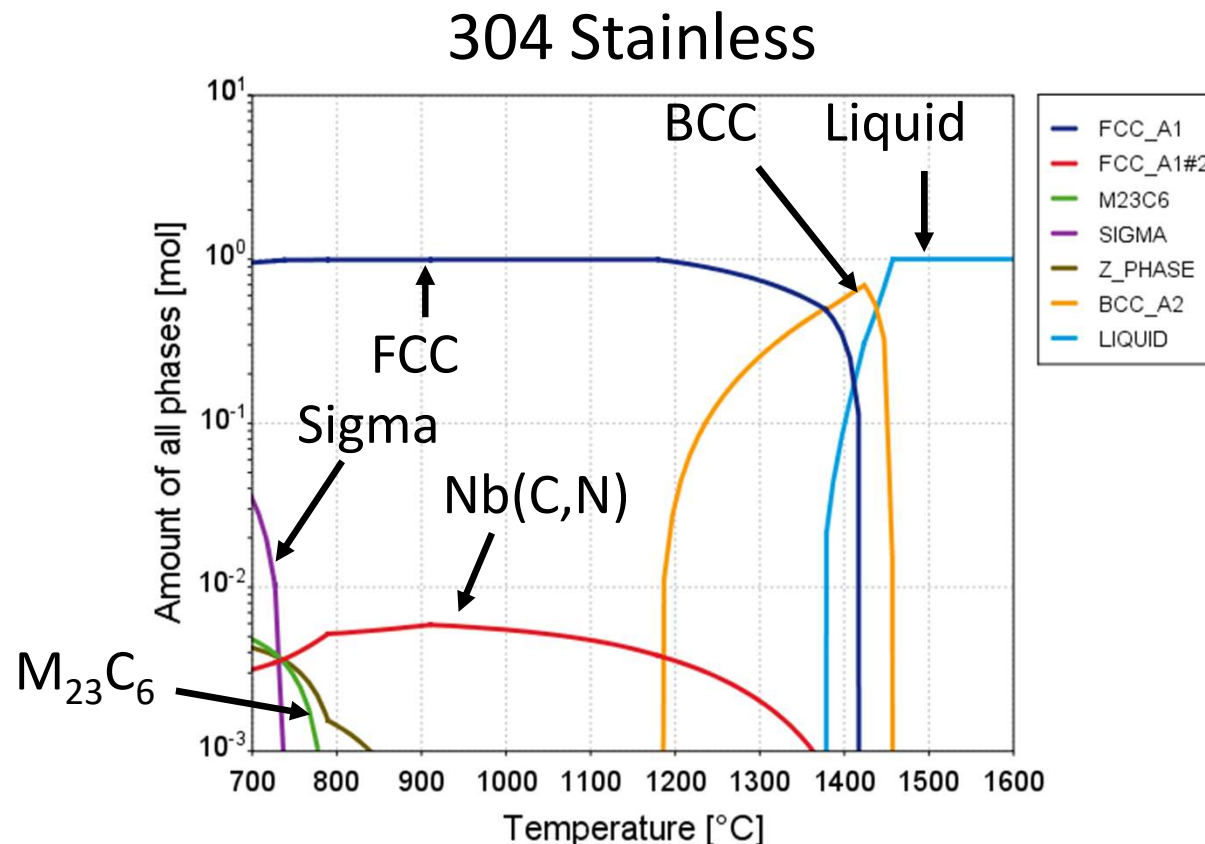
Do I need to append any databases? (i.e. for the gas phase)?

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

One Axis Step Calculations (Property Diagrams)

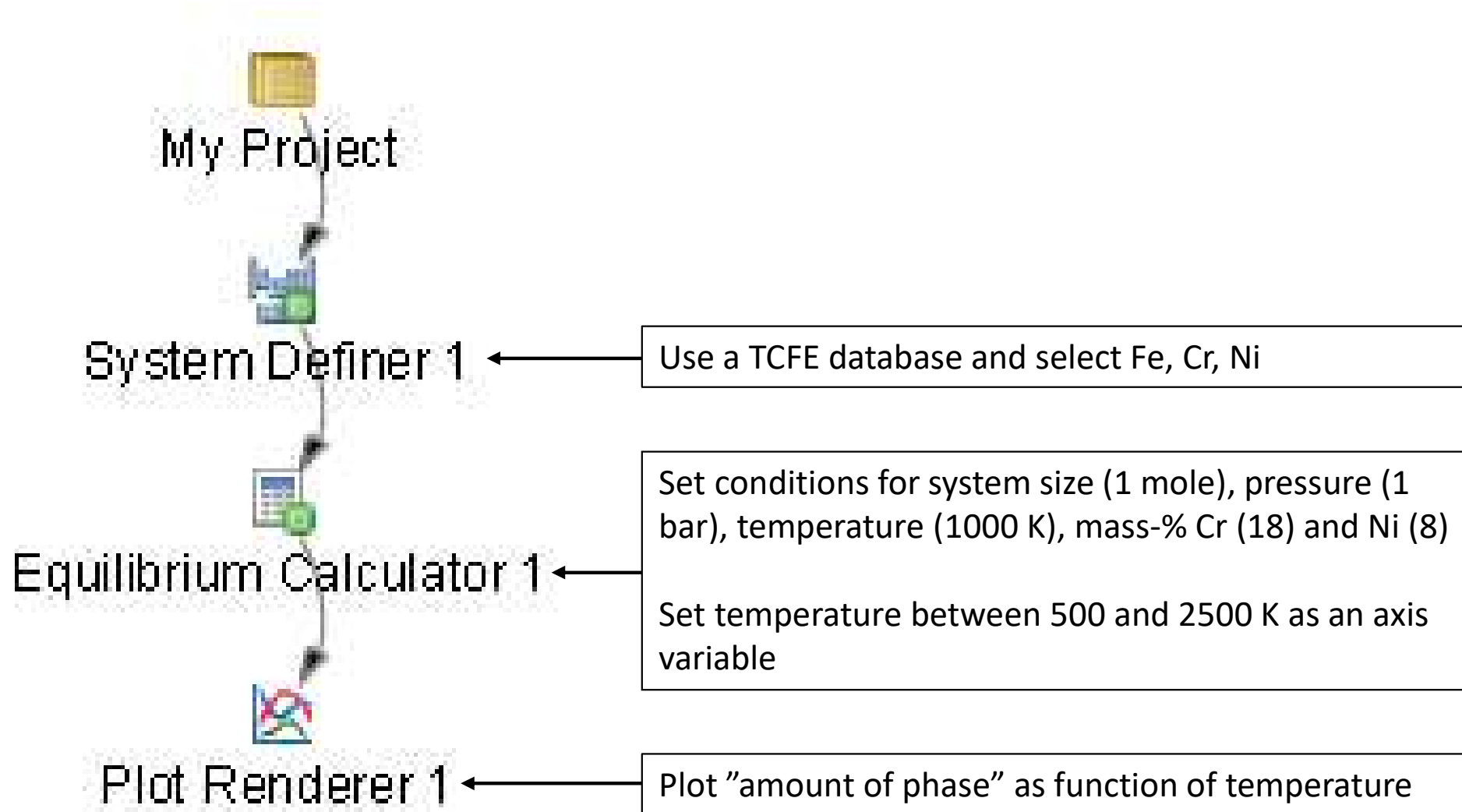
Property diagrams

- ❑ 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.

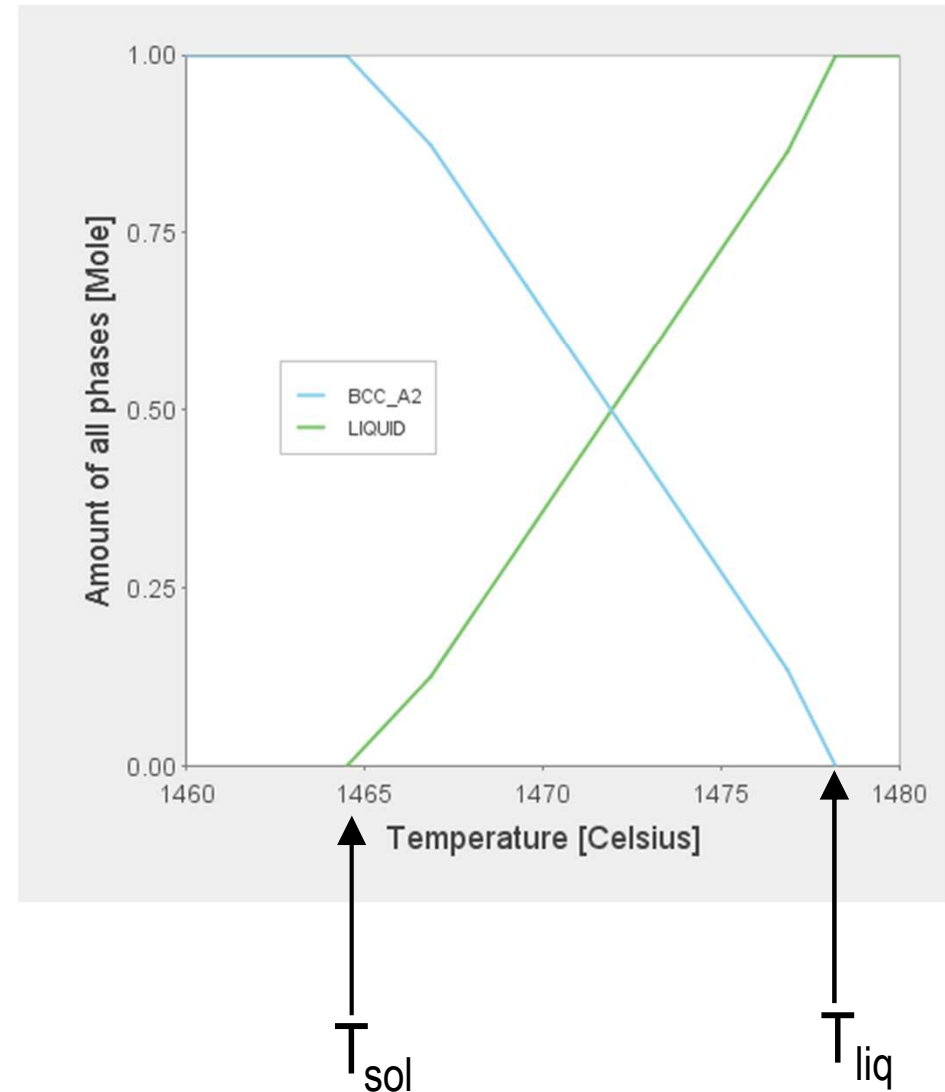
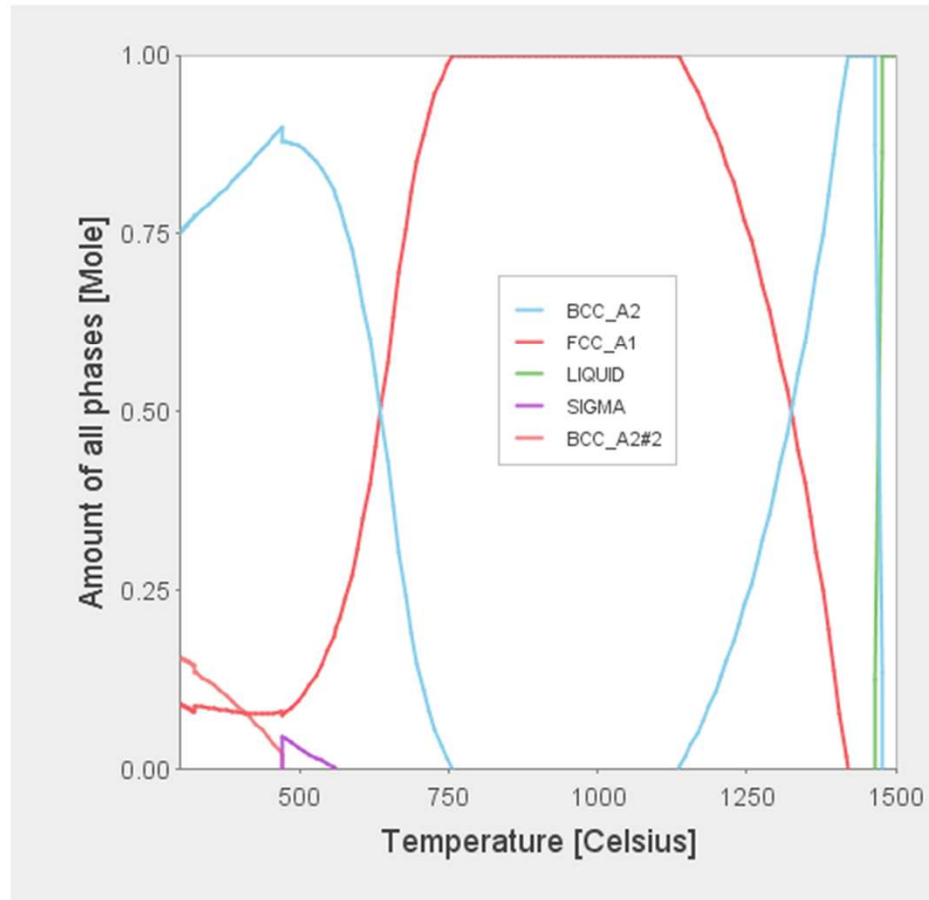


Step in one variable

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



Phase fractions as a function of temperature



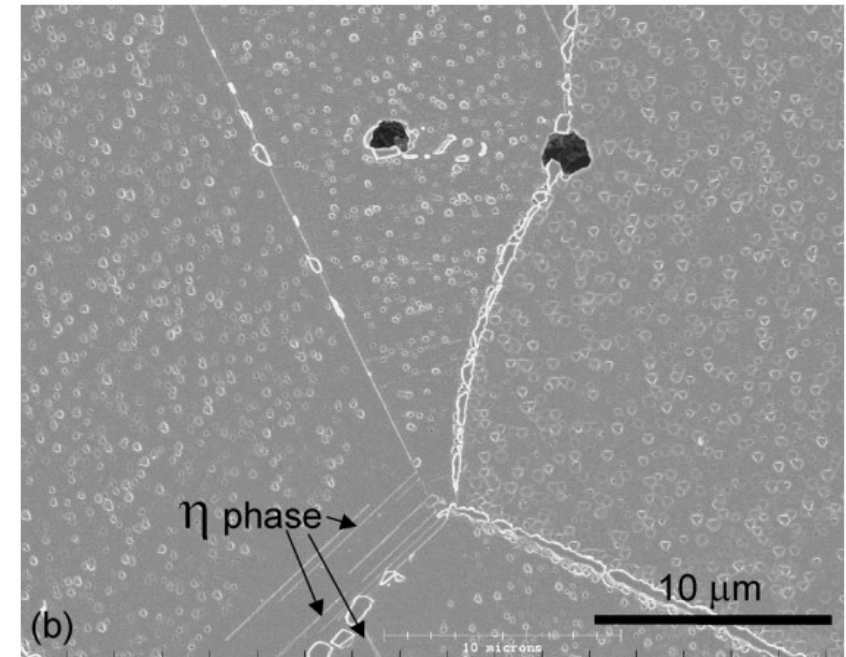
Examples of variables in property diagrams

- ☐ 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

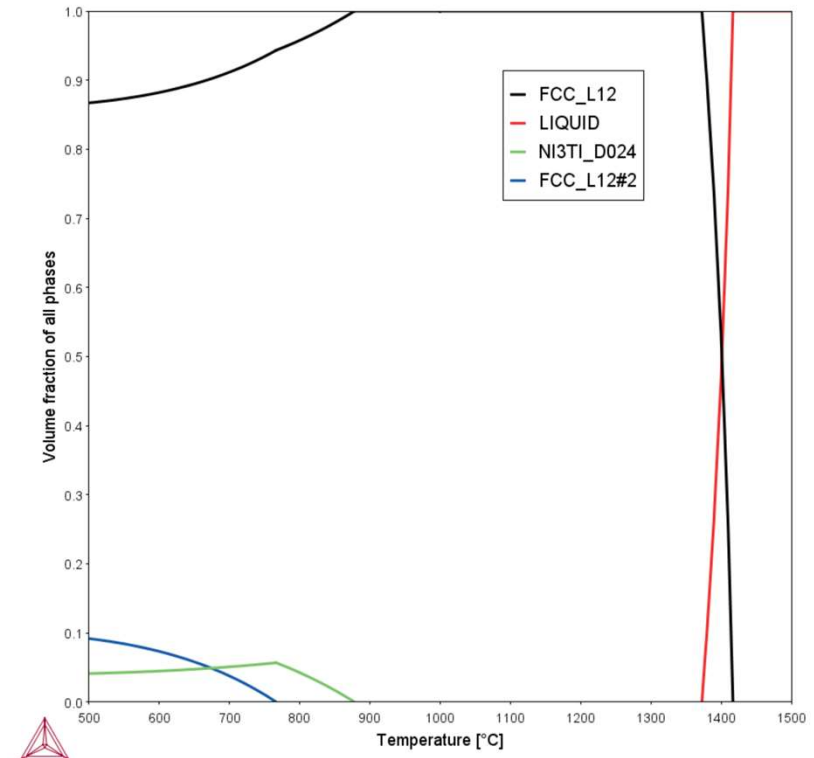
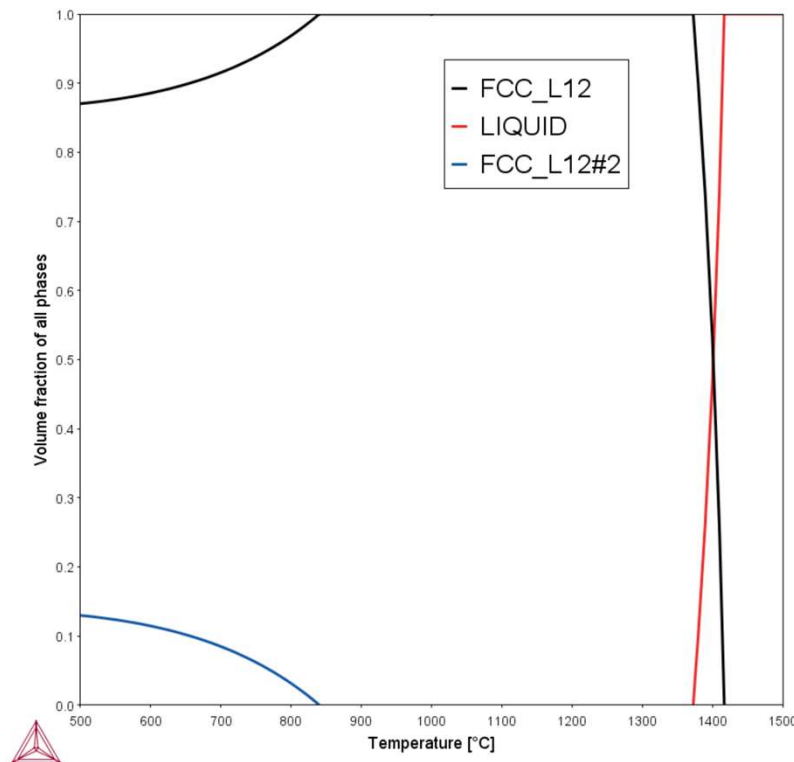
Zhao, J-C., et al., "Phase precipitation and phase stability in Nimonic 263." *Metallurgical and Materials Transactions A* 32.6 (2001): 1271-1282.

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

Calculate a property diagram for a simplified flux:

40 wt-% CaO

20 wt-% SiO₂

5 wt-% CaF₂

15 wt-% MgO

20 wt-% Al₂O₃

Use this composition and step in temperature.

Plot mole fraction of phases in one diagram, composition of the liquid phase in another.

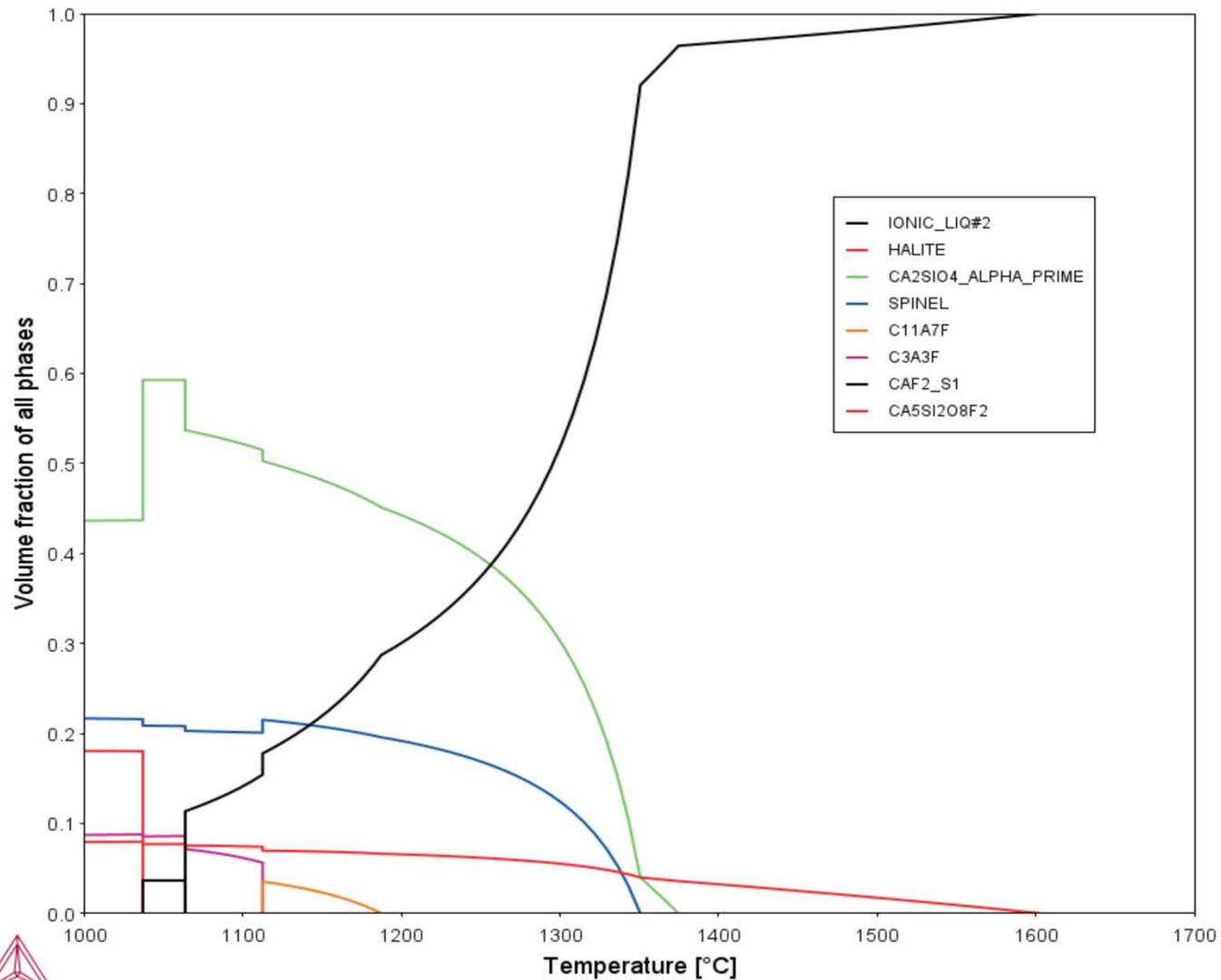
SLAG (or flux) step example 2

– define new components

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TCOX11 : CAO, SIO2, O, CAF2, MGO, AL2O3

Pressure [Pa] = 100000.0, System size [mol] = 1.0, Activity of O2 in GAS = 0.2, Mass percent SIO2 = 20.0, Mass percent CAF2 = 5.0, Mass percent MGO = 15.0, Mass percent AL2O3 = 20.0



Questions & Answers

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!

Tomorrow

Zoom meeting has the same contact details as today.

Same starting time, 09:00 CET (Berlin/Stockholm)

End of Day 1