390 Laboratories

Contents

Lab Demo 1: Materials Selection

1. What is CES/CMS?
   - Cambridge Engineering/Materials Selector
   - Database/Software comes from Cambridge University, UK.

2. Why CMS?
   - Allows off-the-shelf selection of materials (not a software to design new material(s)).
   - There are more than 50,000 materials available to the engineers
     - Q1: "....how one is to find one's way through the enormous catalog, narrowing it down to a single, sensible choice?"

  - Q2: "Can one devise a rational procedure for material selection?"
- Requires minimal knowledge of Materials Science i.e., it can also be used by non-materials scientists/engineers and other professionals.

3. Objectives of Today's Lab. Exercise
   - Demonstration of performance-property link.
   - Demonstration of cross-property plots.
   - Demonstration of multi-level materials selection process.

4. Quantification of Performance and the Performance Index

   In the context of mechanical design, the performance of a component is governed by three factors: the functional requirement (e.g., the need to carry load, transfer heat, withstand shock etc.), the geometry, and the material properties. Then, the performance of component can be expressed by the following relationship:

$$p = f(F, G, M)$$

   where:

   F= specified functional requirements,

   G = geometric parameters,

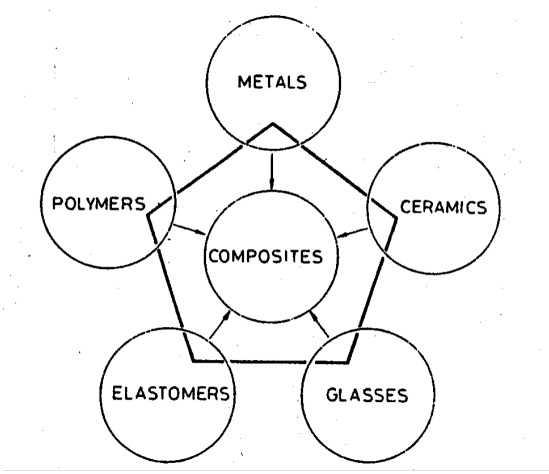
   M = material properties,

   and p is the aspect of the performance to be optimized. The three sets of parameters are assumed to be separable, so the above equation can be written as:

$$p = f_1(F), f_2(G), f_3(M)$$

   where $f_1(F)$, $f_2(G)$, $f_3(M)$ are functions. Since the functions are separable, the optimum material can be chosen without solving the entire design problem. Thus, $f_3(M)$ is called the "performance index". The optimum material is the same regardless of the geometry and functional requirements.

5. Classification of Materials (after M. F. Ashby):



6. Classification of Properties in CMS
    - **Continuous:** General, Mechanical, Thermal, Electrical, Shape Factor
    - **Discrete:** Environment
    - **Logical:** Forming, Joining, Surface Treatment, Available Forms
    - **Identifier:** Metal, Ceramic, Natural, Polymer, Composite
7. Databases in CMS
    - Generic (will be used for lab and homework)
    - Light Alloys Database (purchased)
    - Polymers Database (purchased)
    - Copper Alloys Database (not purchased)
    - Conductors Database (not purchased)
    - Metal Matrix Composites Database (not purchased)
    - Ferrous Alloys Database (not purchased)
    - Foams Database (not purchased)
8. Why Log-Log Plots?
    - When property cross-plots are done, it is found that data for a given class of materials cluster together; they can be enclosed in a single 'balloon'. The wide range of properties for a given

class of material is the manifestation of processing-structure-property links.

- Balloons can be constructed for different kinds of materials representing different properties. Thus, property cross-plot balloons can be displayed in a convenient and accessible way (ease of visualization!).

9. How does it work?

    - Application of set theory and relational algebra

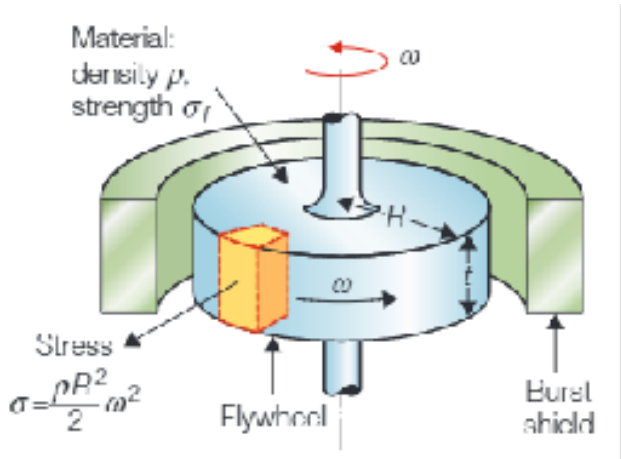
Case Study: Materials for Flywheels (Adapted from CES Background Reading and Tutorial)

Background:

The applications of flywheels to store energy range from children's toys, to old steam engines to the power storage and regenerative braking systems for vehicles.

Advanced flywheel designs have achieved energy densities in the range of 100-250 kJ/kg. Although these energy densities are much less than those in gasoline (44,000 kJ/kg) a sudden release due to failure can be disastrous. Thus, the disk must be surrounded by a burst-shield.

Using CES, we will determine the materials best suited for these advanced flywheel designs. Our selection will be based on maximizing the strength, while minimizing the weight and cost, and maximizing the fracture toughness.



An efficient flywheel stores as much energy per unit weight as possible without failing. The amount of kinetic energy the flywheel can store is limited by its strength. The energy U stored in the flywheel is:

$$U = \frac{J\omega^2}{2} \tag{1}$$

where J is the polar moment of inertia for the disk:

$$J = \frac{\pi}{4}\rho R^4 t^2 \tag{2}$$

The mass of the disk, m, is:

$$m = \pi\rho R^2 t \tag{3}$$

The quantity to be maximized is the energy per unit mass, which we obtain from the combination of the previous 3 equations:

$$\frac{U}{m} = \frac{R^2\omega^2}{4} \tag{4}$$

Spinning the flywheel not only increases the stored energy, but also increases the centrifugal stress. The maximum principal stress in a spinning disk of uniform thickness is

$$\sigma_{max} = \frac{3+U}{8}\rho R^2\omega^2 \tag{5}$$

where ν is Poisson's ratio, equal to about $1/3$ for most solids.

The stress must not exceed the failure stress, σ_f, with an appropriate safety factor, S. These restrictions place an upper bound on the angular velocity, ω, and the disk radius, R. Now (U/m) can be rewritten in terms of the failure stress:

$$\frac{U}{m} = \frac{2}{S\,(3+U)}\frac{\sigma_f}{\rho} \tag{6}$$

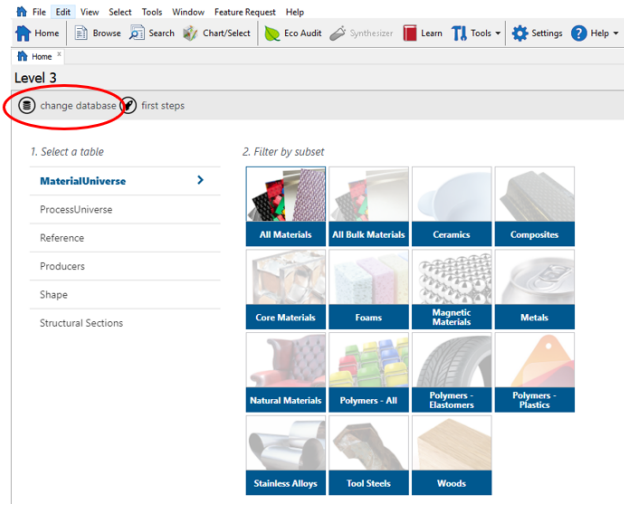
Assuming Poisson's ratio to be constant, the performance index (M) is given as:

$$M = \frac{\sigma_f}{\rho} \tag{7}$$

Thus, the best materials for a flywheel are those with high strength and low density. Additionally, we would like to determine which materials provide the most strength per dollar. Good fracture toughness is also important.

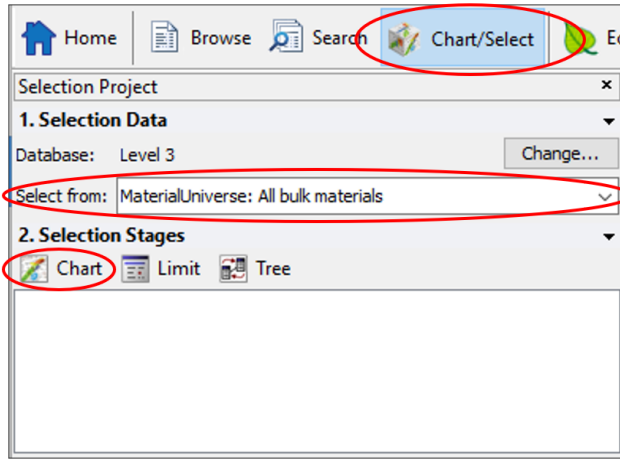
We can now use CES to determine which materials meet these requirements.

- Start CES EduPack
- Select Level 3
- You can change the database by selecting the Change Database option:



Start a new materials selection stage

- Click the "Chart/Select" Button
- Select **All Bulk Materials** under the **MaterialUniverse** tab in **Selection data:**

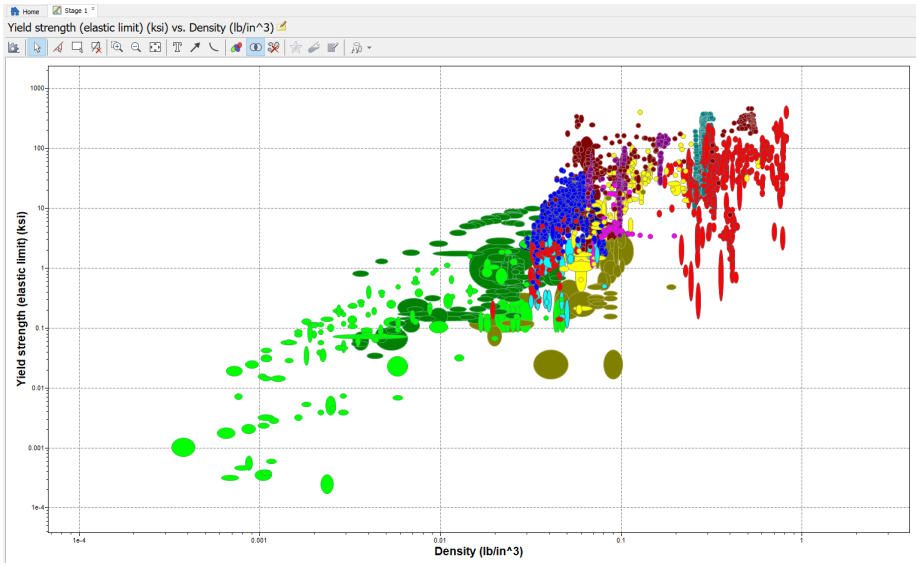


A window entitled "Chart Stage" will appear.

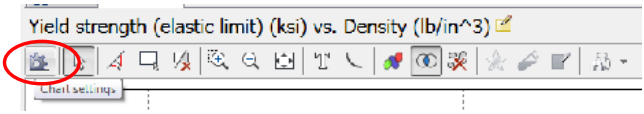
- Click on the Y-axis tab to choose the property for the y-axis.

- Select "Yield Strength (elastic limit)" to set the attribute of the y-axis (Category "Mechanical properties").
  - (You can also select the attributes by clicking on 'Advanced…' and then inserting the property (or combination of properties) you desire to set.)
- Select "Density" to set the attribute of the x-axis (Category "Physical properties").
  - Note that the default scale for the scale is "logarithmic", which is generally what you want.
- click on "OK" in the Chart Stage dialog box.

After a short pause, the program will plot a materials selection chart in the Stage 1 window:



Because the properties of most materials cover a very wide range of values, it is almost always desirable to plot the charts with log scales. This is the default for CES. You can change the scales to linear and back again by clicking on the Stage Properties button (indicated below) in the toolbar and clicking on the X-axis and Y-axis tabs to change the scales. Leave the scales on the 'Logarithmic' option for the purpose of this exercise.

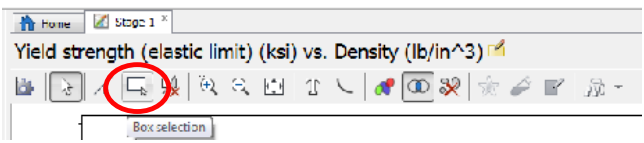


In a graph setting only one axis is also allowed. This axis could plot a combined property corresponding to a performance index ($\sqrt{E}/\rho$, for example), but it is generally more useful to plot the properties against one other in order to get a better visual representation of the full property space.

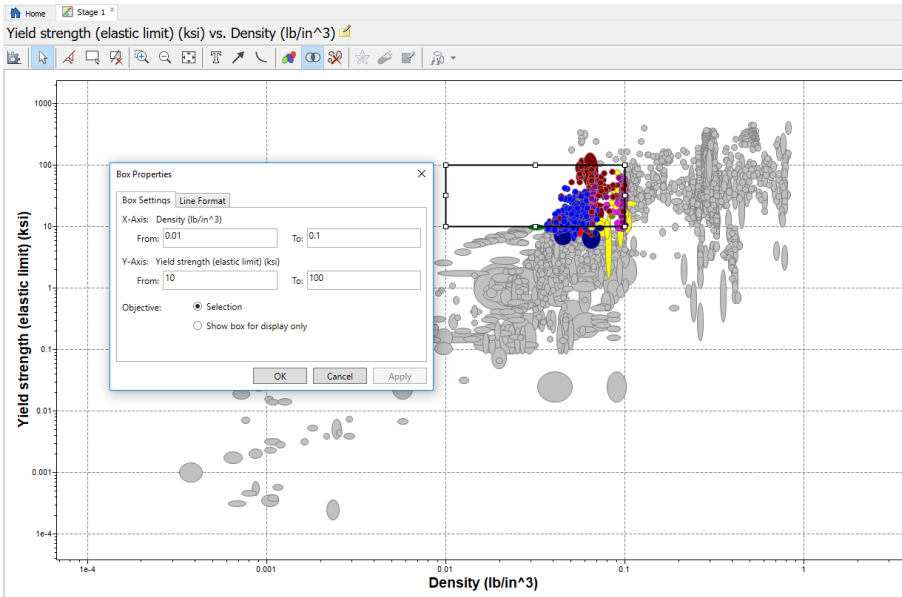
Selecting a subset of materials in a box

The simplest way to select a subset of materials from the chart is to draw a 'box' around the ones you want. The procedure for doing this is as follows:

- Click once on the "Box Selection" button on the main toolbar above the graph:



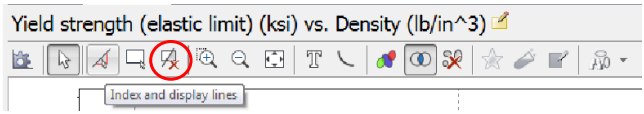
- Specify the area of the selection box by defining the positions of two opposite corners. Select the materials within the ranges: (note: To change the units select – Tools > Settings > Units). In this example use 0.01 lb/in^3<Density<0.1 lb/in^3, and 10 ksi<Elastic Limit<100 ksi.
  - Note the cursor coordinates appear at the bottom left of the screen to aid you.
  - Click on the point(x,y) = (0.01, 10), and hold the mouse button down.
  - Drag the cursor to the point (0.1, 100), then release the mouse button.
  - To be more precise, right-click the box, select "Properties" and input specific values in the "Box Settings" tab:



The materials in the box and all the materials that cross the boundary of the box are now plotted in color. This indicates that they have been included in the current subset of materials - they have 'passed' the selection stage. Materials failing the selection stage are plotted in gray. To hide the failed materials, click "Hide failed records" button.

You can change your selection at any time by re-sizing the box:

- Click on one edge of the selection box, square handles will appear at each corner
- Click on one of the handles and hold the mouse button down
- Drag the corner of the box to a new position and release the mouse button
- To be more precise:
  - Right Click the box, and select "Properties".
  - Input boundary values in "Box Setting" tab.
- To remove the selection completely, click on the "Delete lines and boxes" button.



Use of performance indices

A better way to select a material for a flywheel is optimize the strength to weight ratio of the material, *i.e.* use the performance index, M, defined early (see Eq. 7):

$$M = \frac{\sigma_f}{\rho} \tag{8}$$

Taking the logarithms of both sides of this equation we obtain:

$$\log M = \log \sigma_f - \log \rho \tag{9}$$

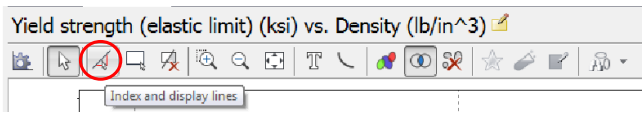
Re-arranging:

$$\log \sigma_f = \log M + \log \rho \tag{10}$$

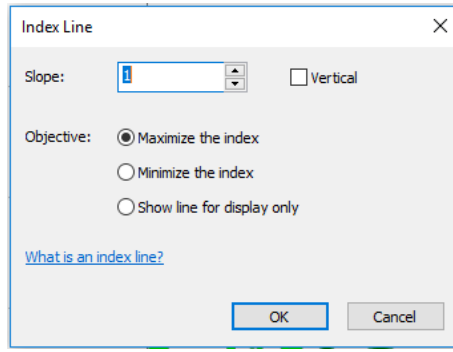
This equation can be plotted as a line of slope 1.0 on a log-log plot of σ_f vs. ρ. All materials lying on this line have the same value of M, and therefore, are equally good for a flywheel. Materials above the line have a higher value of M and perform better.

To select a subset of materials with a high value of M, do the following:

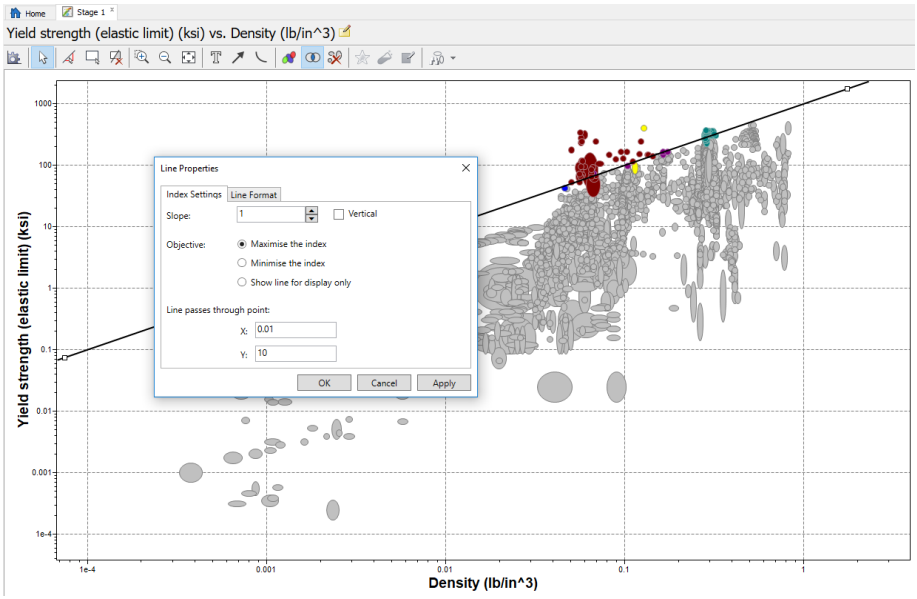
- Click once on the Index and Display lines button on the toolbar:



The program will now present you with the dialog box Index Line:



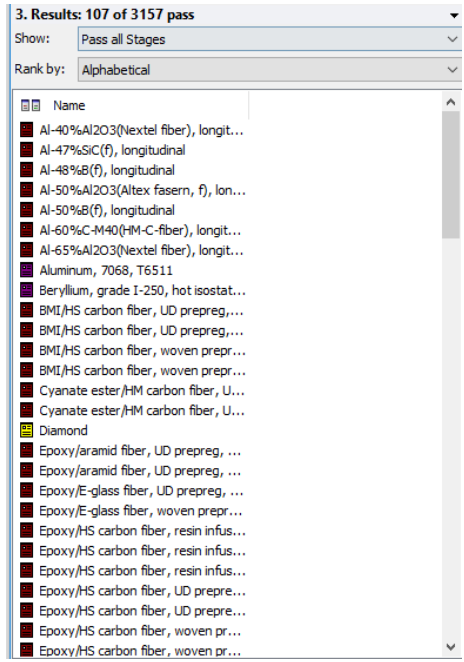
- Input Slope value 1.
- Select "Maximize the index".
- Click on OK.
- Now pick the point on the chart where the density is 0.01 lb/in3 and the elastic limit is 10 ksi:
  - Click once on the chart to display the line
  - Right click the line and select "Properties"
  - Input the point value (X: 0.01, Y: 10) that the line to passes through
  - Click on OK
- The program now displays a diagonal line of slope 1 through (0.01, 10). The line corresponds to$M = 1000\,\text{ksi}/\left(\text{lb}/\text{in}^3\right)$.



Note that all the materials above the line and crossing it are plotted in color; they 'passed' the selection. All the materials below the line are plotted in gray; they 'failed' the selection.

View Intermediate Results

Use the Results window to view the results of your selection. It is located on the bottom-left of the screen:



The contents of the Results window show that 107 out of 3157 materials in the MaterialsUniverse database passed the stage 1 selection (results may be slightly different, depending upon the exact position of your selection line and your version of the database). Double-clicking on any of the materials in the results list will make its bubble flash on the selection chart and will send information about it to the Properties window.

Moving a Selection Line

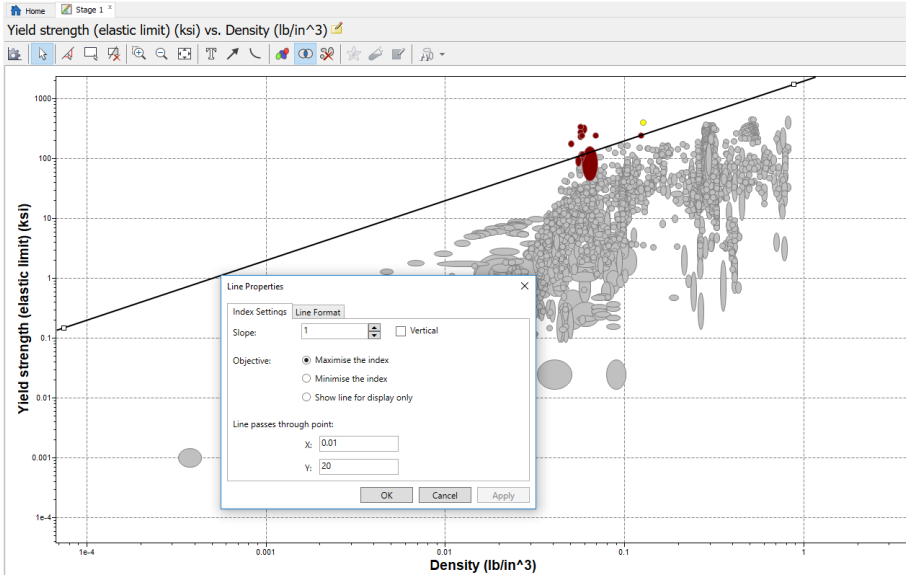
The selection line can be easily moved to tighten the selection criteria as follows:

- Click once on the selection line and hold the mouse button down.
- Move the mouse to a point near (0.01, 20), (Density=0.01 lb/in^3, elastic limit=20 ksi), then release the mouse button (the value is showed at lower-left corner of the window).

Alternative Method (easier and more accurate):

- Right click the line and select “Properties”.

- Input the point value (X: 0.01, Y: 20) that the line to passes through,
- Click on OK.



The selection will update automatically, and the Results window will reflect the changes.

- For the purposes of this lab, revert back to original selection (line passing through (0.01, 10)).

Zoom

Using Zoom is very similar to selecting a material subset within a box. You simply select two sets of points at opposite corners of the area of interest.

- Click once on the "Zoom in" button on the main tool bar.
- Click once on point (0.01, 10) on the chart, and hold the mouse button down.
- Drag the cursor to (0.1, 100) on the chart, then release the button.

To return the chart to full size, use the Autoscale button on the zoom tool bar (the button with the crossed magnifying glass).

Identifying a Particular Material

To identify a particular bubble on the materials selection chart:

- Click on the arrow button and then on a material bubble on the selection chart/

The bubble will now flash on and off, and a temporary label will appear on the screen. When you double click on a material, the property information pops up in the Properties window. The Properties window will now display the properties of the material that you selected on the chart.

To see the bubble corresponding to a material in the pass/fail table or search results, right click on the name and select "Highlight" or "Label". You'll get it labeled. You can also change the color of bubbles.

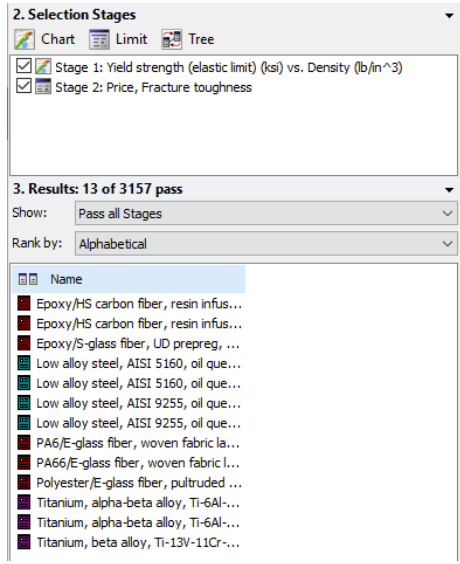
Creating a Second Stage of Selection

Now that you have successfully selected materials with a high strength-/density ratio, it is necessary to consider other aspects in flywheel design, such as price and fracture toughness. Begin a second stage of selection:

- Start a new selection stage by clicking "Limit" in Selection Stages.
- Input 30 for the minimum value for "Fracture toughness" (Impact & fracture toughness), and 10 for maximum value for "Price" (Price).
- Click Apply.

Results

Having performed two independent selection stages, it is useful to find out which materials have passed both stages. The Results window has a drop-down list. The default contents of the Results window are materials passing 'All stages' in the drop-down list. 'All stages' means the materials that have passed all selection stages performed so far. It can be seen that 13 materials out of 3157 achieved this:



There are various other format options in the Results window. Suppose we wish to find out about the materials that passed one of the two selection stages. Find these as follows:

- Select 'Pass/Fail Table' from the drop-down list at the top of the Results window.

Symbols '✓' and 'x' on the right side of the window stand for 'Pass' and 'Fail'. Cold worked tool steels passed stage 1 but failed stage 2; conversely wrought austenitic stainless steels failed stage 1 but passed stage 2.

To view the materials that only passed Stage 1 or Stage 2:

- Select 'Stage 1' or 'Stage 2' from the list at the top of the Results window.

Saving Results

- Select 'Save Project' from the File drop down menu.

Some Notes on Power Laws and Units

Some aspects of this example were pretty easy to sort out because the power law exponent in the Ashby plot was 1. In other cases you'll have power laws of 0.5, 2, 1.2 or other more complicated variants. The units of the performance index in cases like this get pretty strange and can add to a lot of confusion. Consider, for example, the relatively common situation where the performance, M is equal to $E^{1/2}/\rho$. It's relatively straightforward to work out the slope of line on the Ashby plot that corresponds to materials with the same performance index. In this case if we plot $\log \rho$ vs. $\log E$ the slope is 0.5, and if we plot $\log E$ vs. $\log \rho$ the slope is two. Because all points along the line have the same value of the performance index, we can specify this quantity by specifying any combination of E and ρ that lie on this line. Suppose for example, the line goes through a point where $\rho = 1000\,\mathrm{kg/m^3}$ and $E = 10^9$ Pa. Then the performance index of the material in this case is:

$$M = \frac{\left(10^9\,\mathrm{Pa}\right)^{1/2}}{1000\,\mathrm{kg/m^3}} = \frac{\left(1000\,\mathrm{Pa}\right)^{1/2}}{\mathrm{kg/m^3}} \tag{11}$$

In the CES EduPack software we specify the same value of M by pairing $E = 1000$ Pa with ρ=1 kg/m^3, or by pairing $E = 10^9$ Pa with ρ=1000 kg/m^3. If we want to enter the performance index corresponding to a specific line into a plot generated by CES EduPack, we enter the most convenient combination of values.

Lab 2: Calculation of Phase Diagrams and Driving Force Using Thermo-Calc 2021b GUI

ThermoCalc Overview

1. What is Thermo-Calc?
    - Software/Database package for thermodynamic calculations
    - Originated from Royal Institute of Technology, Stockholm (www.thermocalc.com)
2. What Thermo-Calc does?
    - Stable and meta-stable heterogeneous phase equilibria

- Amounts of phases and their compositions
- Thermochemical data such as enthalpies, heat capacity and activities
- Transformation temperatures, such as liquidus and solidus
- Driving force for phase transformations
- Phase diagrams (binary, ternary and multi-component)
- Solidification applying the Scheil-Gulliver model
- Thermodynamic properties of chemical reactions
- Consider constrained equilibrium, such as effect of stress, interfacial energy etc.

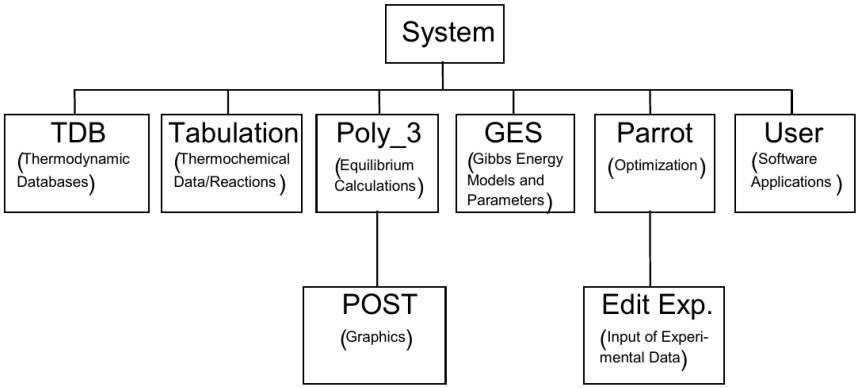
3. Applications
    - Materials processing
    - Materials design

Objectives

1. How to use Thermo-Calc 2021b (Graphical Mode)
2. How to interpret the results of a single equilibrium calculation
3. Calculation of multi-component systems
4. Calculation of driving force for precipitationis Modular

Modular Character of Thermo-Calc

The organization of Thermo-Calc modules is schematically shown below:



Definitions (and Reminders) Relevant to Thermo-Calc

System:

A region (defined in terms of composition, temperature and pressure) of interest that can be closed or open to the exchange of matter, heat and work to its surroundings. In ThermoCalc all equilibrium calculations are performed with the assumption that the system is closed.

Phases: A region in the system that is homogeneous (uniform) and physically distinct and has the same structure and property everywhere.

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

Gibbs Phase Rule: States 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 to describe a given phase.

Constituents: Determine the composition dependence of the properties of the phase and can reflect additional internal degrees of freedom.

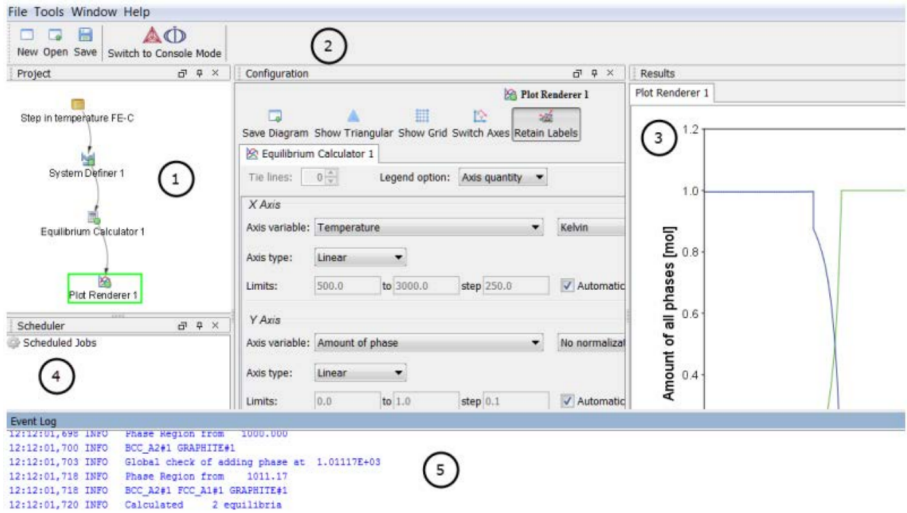
Species: The collection of all constituents for the phases in a given system and can be elements, molecular aggregates, charged or neutral.

Thermo-Calc 2021b Graphical User Interface

TC2021b has a Graphical User Interface as well as an optional Console Mode. The software allows for calculations of multicomponent phase diagrams and property diagrams through the use of menus, buttons, and entering a few values e.g. compositions. In this lab, only Graphical Mode will be used. TC2021b-GUI uses the same thermodynamic databases as previous versions of Thermo-Calc and Console Mode.

The figure below is an example of the default GUI layout for Graphical Mode.

1. **Project:** Create, manipulate and navigate between the activities that make up a project.
2. **Configuration:** Shows the settings that can be configured for the currently selected activity.
3. **Results:** Shows the results of a calculation, either plotted as a diagram or displayed in table format.
4. **Scheduler:** Displays information about jobs, such as calculations, that are being performed or are scheduled to be performed. You can cancel scheduled jobs and if a job has failed, then you can view information about the error.
5. **Event log:** By default, this window is closed but it displays during calculation processes. You can always open it to view progress of calculations and to troubleshoot.



Basic Steps in a ThermoCalc 2021b (Graphical Mode) Calculation

1. Create a Project: Select the desired application module in the main window
2. System Definer: Define the database and system
3. Equilibrium Calculator: Define the conditions for the initial equilibrium
4. Perform: Calculate the equilibrium and extrapolate it by stepping/mapping in 1 or 2 directions
5. Plot/Table Renderer: Define the axes to plot

Important Concepts in Thermo-Calc

1. Status

   Entered: The phase, component, or species can freely participate in the energy minimization procedure.

   Dormant: The phase is allowed to participate in the energy minimization but not allowed to have any mass (i.e. driving force).

   Fixed: The phase is forced to be present in a given quantity

   Suspended: The phase, component, or species is ignored.

2. The Conditions of Equilibrium

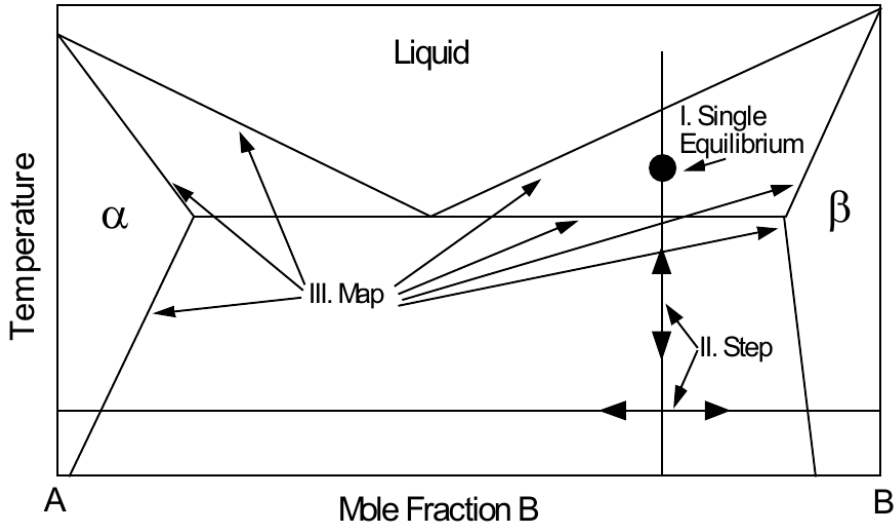
    - The system must be constrained by intensive or extensive state variables in order to reduce the degrees of freedom in the system to zero.
    - The degrees of freedom in the system are equal to the number of components plus 2 (temperature and pressure).
    - Any phase that is forced to be present by a FIXED status reduces the degrees of freedom by 1.
    - Typically the size of the overall system must be constrained by setting the number of moles in the system equal to 1.
    - Functions of state variables can also be used as conditions, but must be posed such that the function equals 0.

3. State Variables

- Intensive:
    - T = Temperature in K
    - P = Pressure in Pascal
    - ACR(component) = Activity
    - MUR(component) = Chemical potential
- Extensive:
    - S, S(phase) = Entropy of the system or phase
    - V, V(phase) = Volume of the system or phase
    - G, G(phase) = Gibbs energy of the system or phase
    - H, H(phase) = Enthalpy of the of the system or phase
    - A, A(phase) = Helmholtz energy of the system or phase
    - DGM (phase) = Driving force per mole of the phase/RT
    - N(comp), N(phase, comp) = Number of moles of the component in the system or phase
    - B(comp), B(phase, comp) = Mass of the component in the system or phase
    - N = Total number of moles in the system
    - B = Total mass in the system.

All extensive variables can be normalized to the moles in the system by appending an M to the descriptor. The same is true for the mass with W and the volume with V. As a convenience X and W can be used to denote mole fraction and mass fraction respectively.

Types of Calculations in POLY3 Module

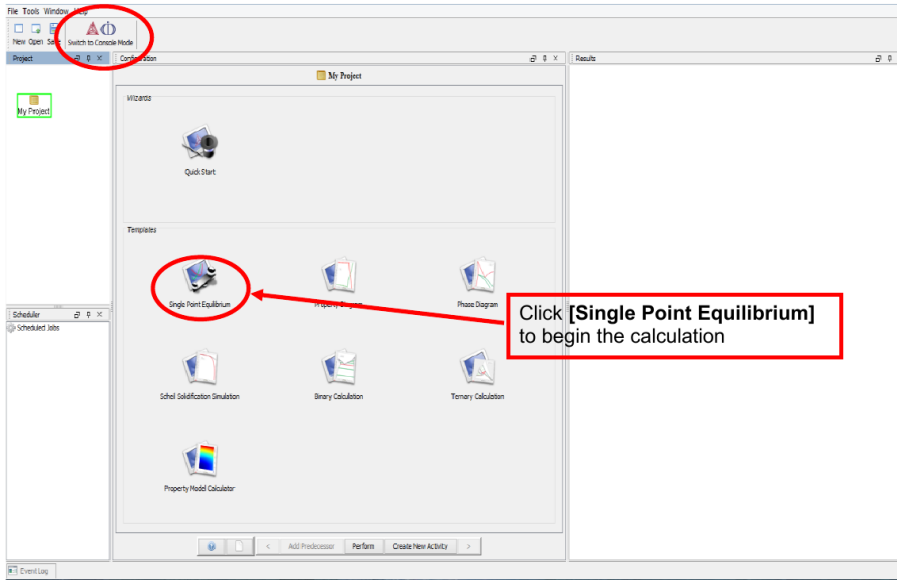


- I. Single Equilibrium (Single Point Calculation): Nothing is varied
- II. Step Calculation (Property Diagram): One state variable is varied
- III. Map Calculation (Phase Diagram): Two state variables are varied

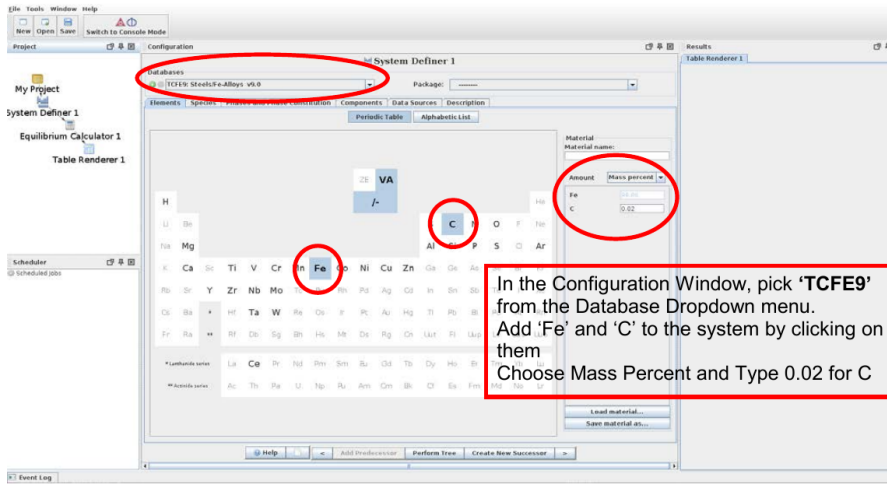
EXAMPLE 1: Single Point Calculation of Fe-0.02C (wt%) at $T = 800\,^{\circ}$**C**

You can use the Single Point Calculation to determine phase fraction and composition. Its results should match what you could calculate from Lever Rule.

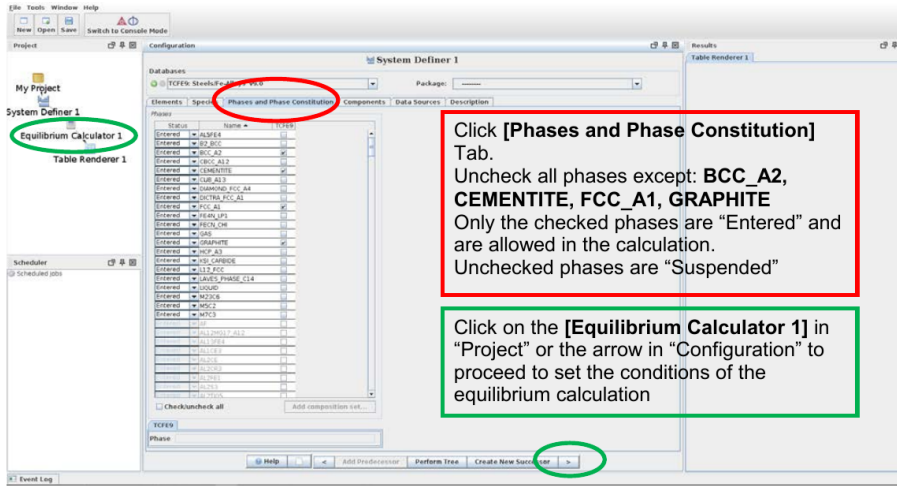
1. Open TC2021b and enter GUI mode. Select 'Single Point Equilibrium'



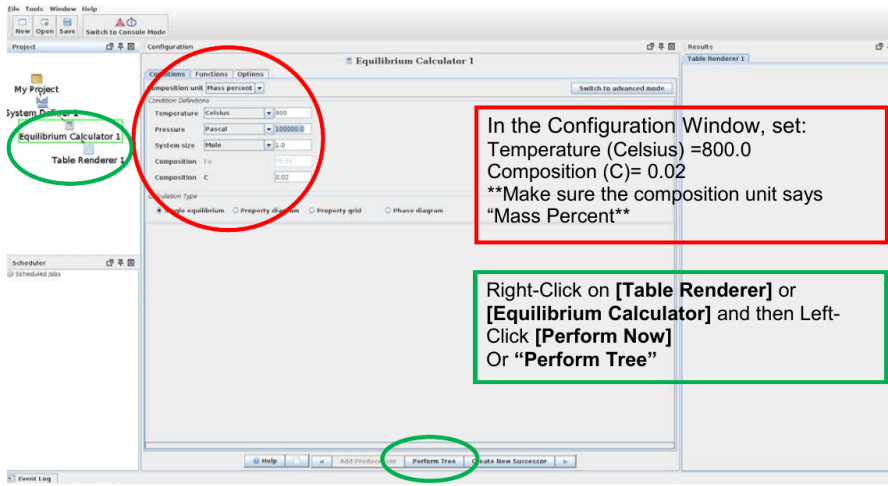
2. System Definer 1 - Pick Database and Elements in System



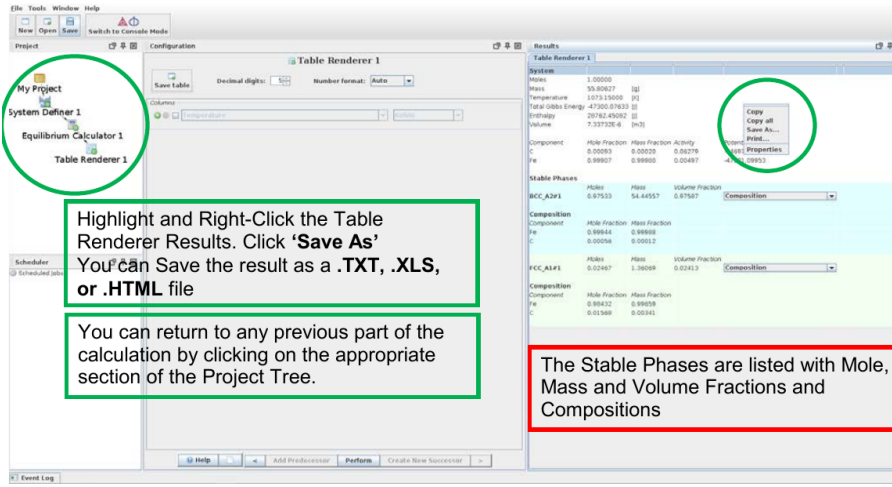
3. System Definer 1 - Identify Phases and Phase Constitution in System



4. Equilibrium Definer 1-Set Temperature and Composition. Then Perform calculation. The calculation would take a few seconds.



5. Table Renderer Results and Save as a Text, HTML or XLS file



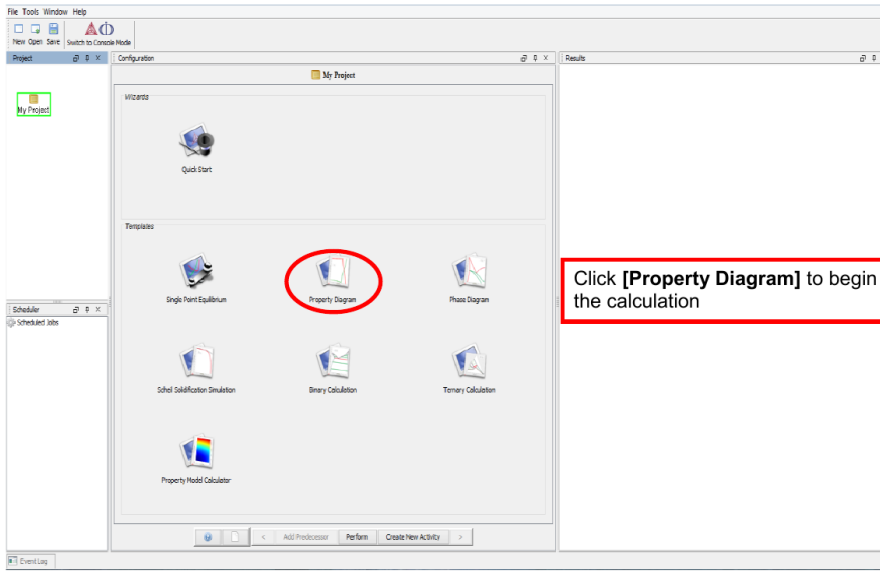
EXAMPLE 2: Step Calculation for a Dilute Al-Mn-Ge-Si Alloy

Property Diagram starts a "Step" calculation. This involves "Stepping" through a single variable after initiating a point equilibrium. Step Calculations can result in graphs or tables of the calculated properties. For example, to determine the optimum temperature for processing for a given alloy we can use one of the compositions as variable for stepping.

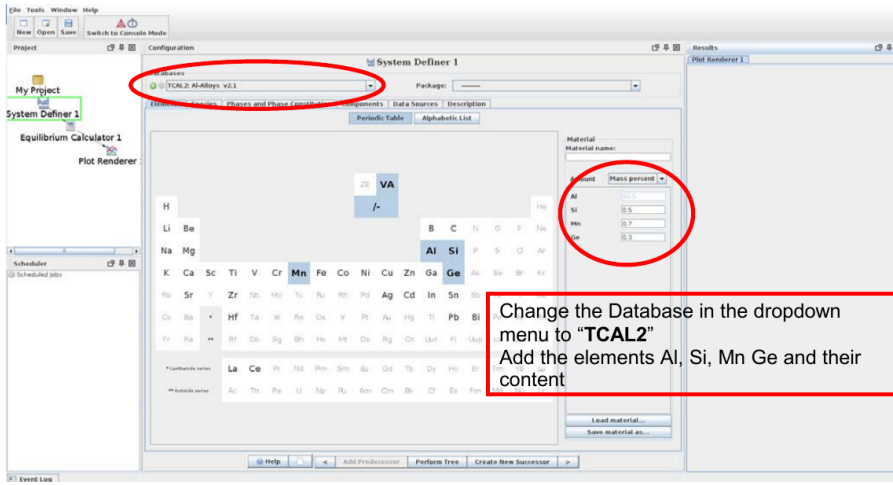
In this example, we will use an Al-0.7Mn-0.5Si-0.3Ge (wt%) alloy. We want to find out what is its solution treatment temperature (i.e., the temperature at which all solutes are dissolved in Al). We also want to know what the equilibrium phase(s) are at various aging temperatures.

1. Open TC2021b and enter GUI mode. Select 'One Axis Equilibrium'

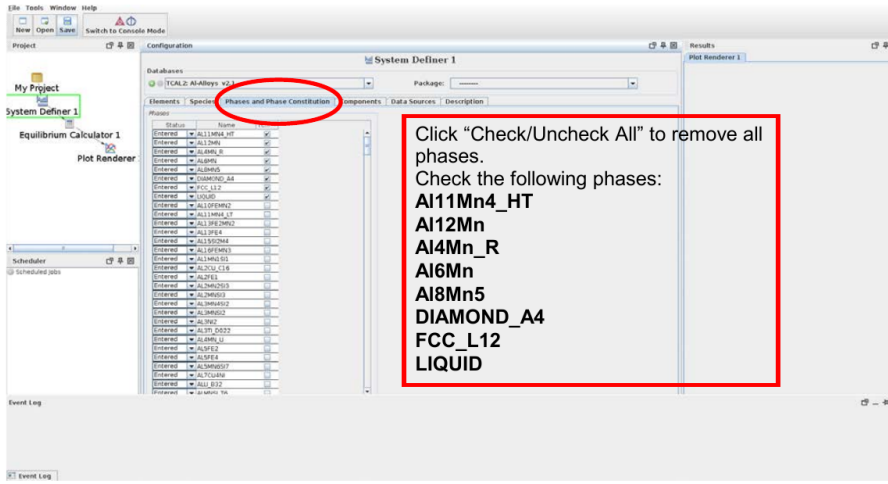
Step 1: Open TC2017b and enter GUI mode. Select 'Property Diagram'



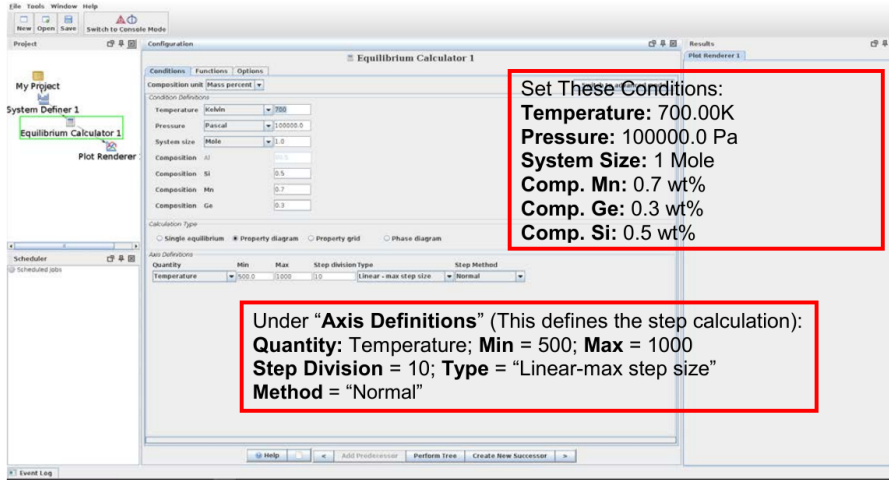
2. Change the database, add the correct elements, go to the Phases tab.



3. Choose Phases.

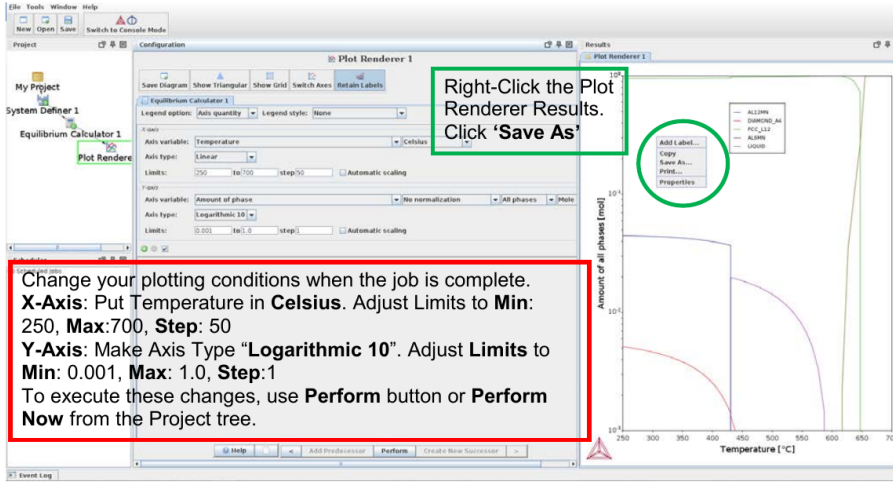


4. Set Conditions (Temperature and Composition). Then Perform calculation.

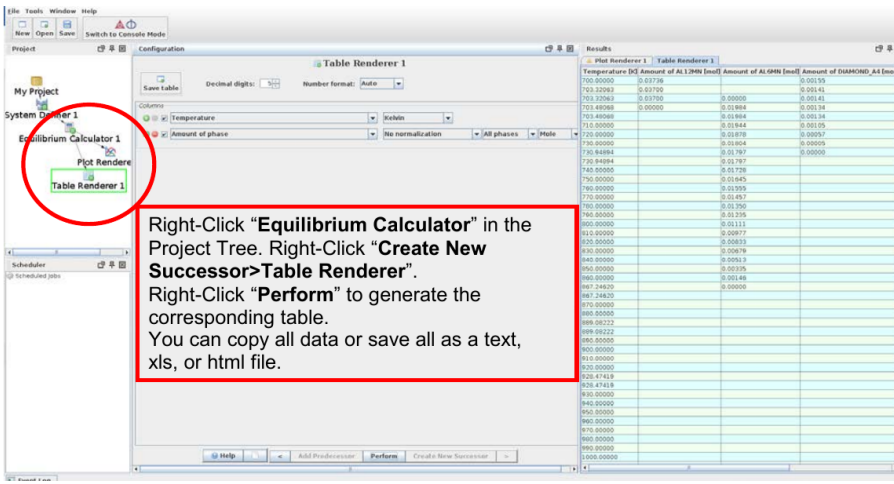


5. Plot Renderer Results and Save the Diagram or Data Table.

   This is commonly called a Step Diagram. It shows equilibrium phase fractions of phases present in the system at a given temperature. It is best to plot phase fraction in Log base 10.



A table with the data calculated can be created using "Table Renderer".

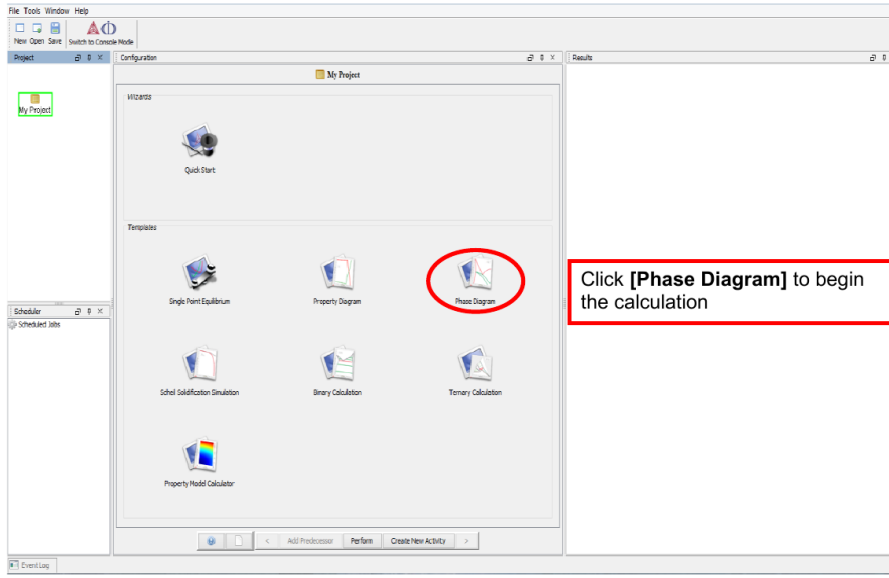


EXAMPLE 3: Map Calculation for a Fe-C Metastable Phase Diagram

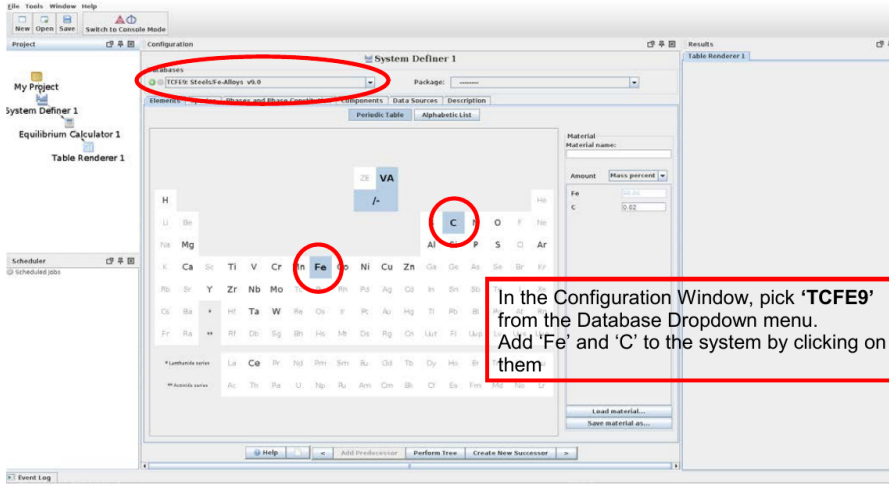
Mapping Calculations allow variation of two variables. These enable the calculation of phase diagrams (varying Temperature and Composition). For this example, we'll calculate a metastable equilibrium diagram of Fe-C.

1. Open TC2021b and enter GUI mode. Select 'Phase Diagram'.

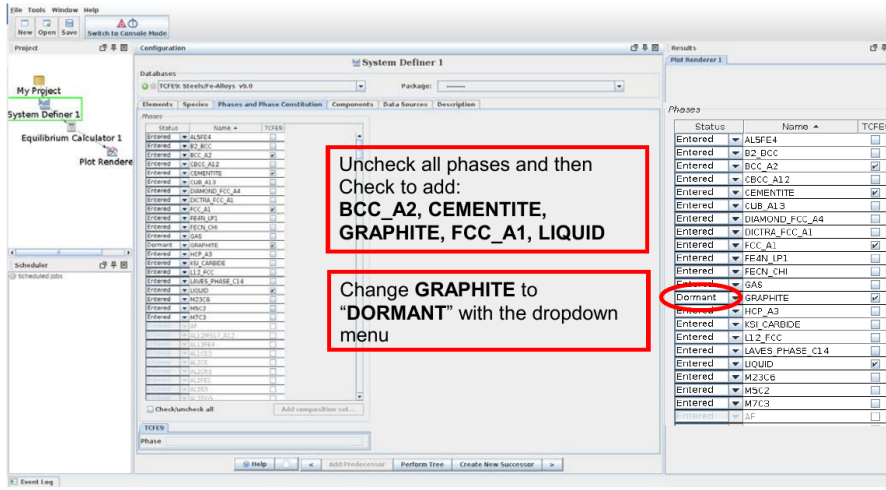
Binary Calculator or Ternary Calculator are quick templates for Binary and Ternary Diagrams but feature less customizability.



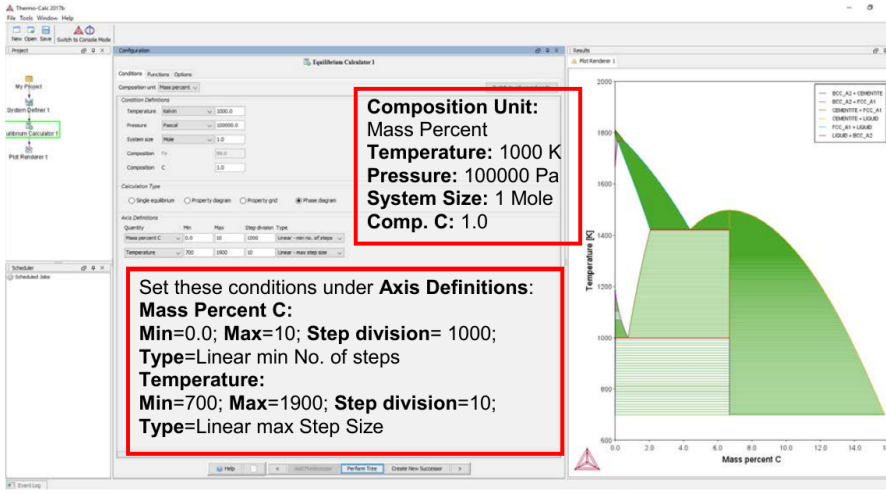
2. Choose the Correct Database and add Elements



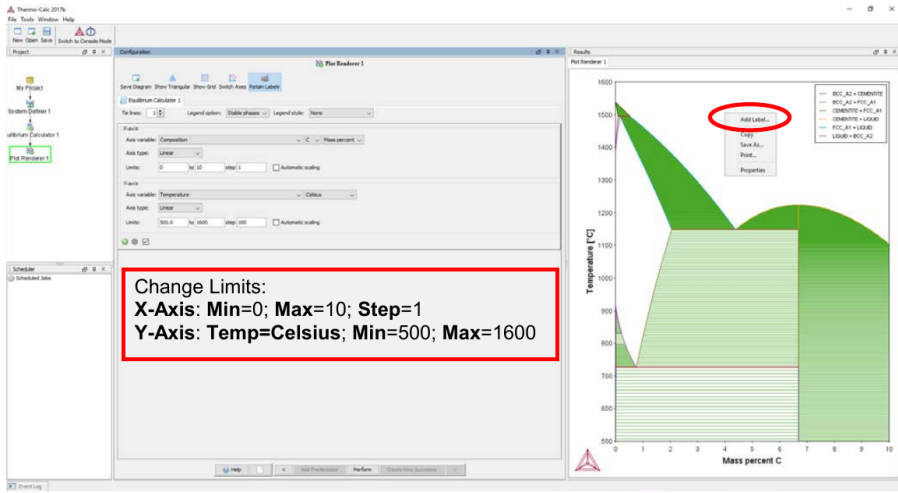
3. Add Phases and Make Graphite Dormant



4. Set Mapping Conditions, Then Perform calculation

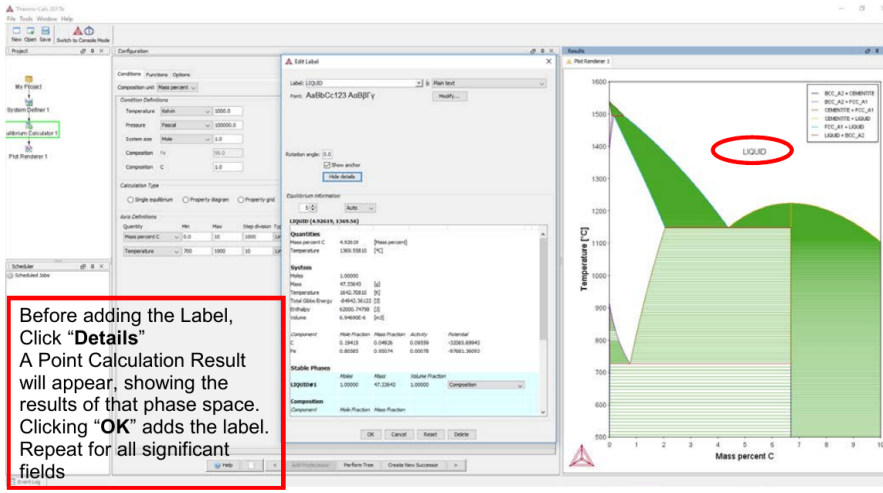


5. Change Axis Limits. Insert Labels.



6. Label Phase fields.

   This is a metastable equilibrium diagram due to Graphite. The only accurate section is that with less than 10 wt% C.

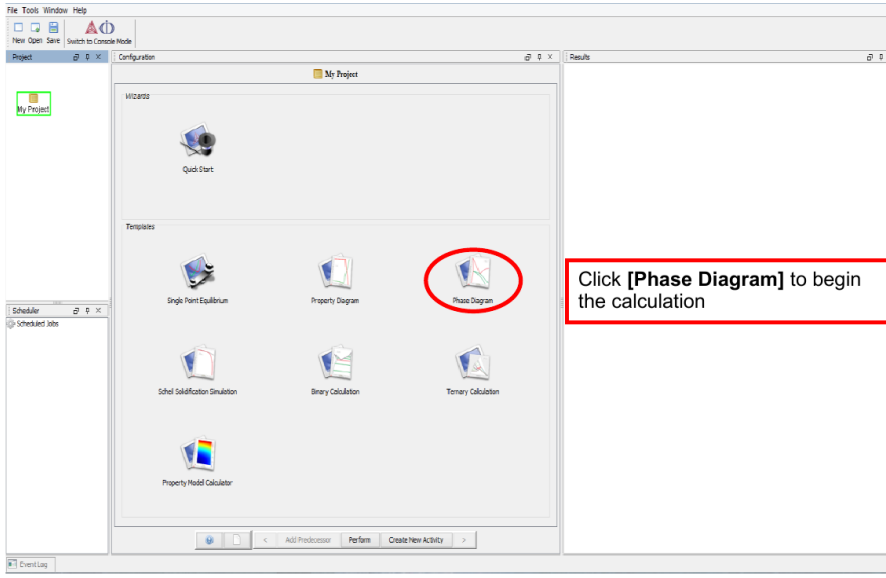


EXAMPLE 4: Calculate an Isothermal Section of Fe-Ni-Cr system at 600 °C

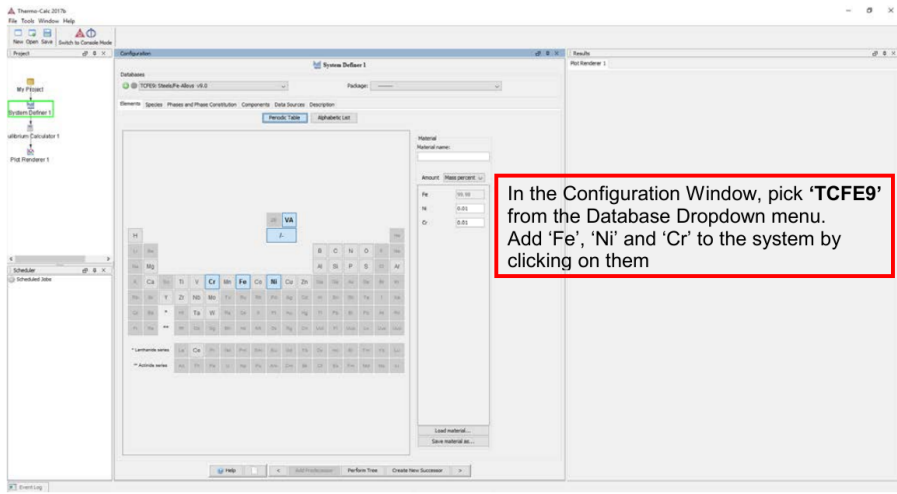
An isothermal section of the ternary system provides us the composition-phase roadmap at a particular temperature. This informa-

tion is very useful in selecting alloy compositions, knowing the equilibrium phases present, their amounts and compositions for a given alloy composition etc. The phase equilibria of Fe-Ni-Cr system is the basis for designing various types of stainless steels. For example, if one wants to design an austenitic stainless steel, the alloy composition should be in the FCC phase field. Or, if one wants to design a duplex stainless steel, the alloy composition should be in the BCC+FCC phase field. Calculation of an isothermal section at 600°C is a demonstration of such alloy selection process.

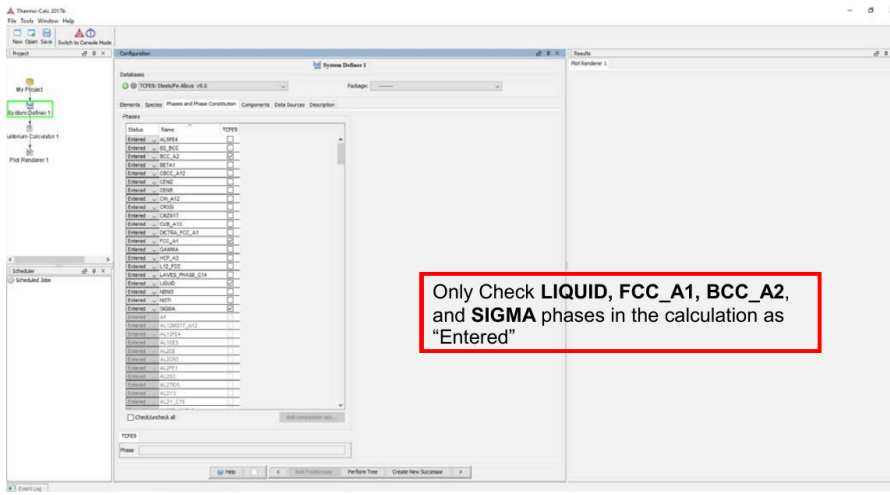
1. Open TC2021b and enter GUI mode. Select 'Phase Diagram'



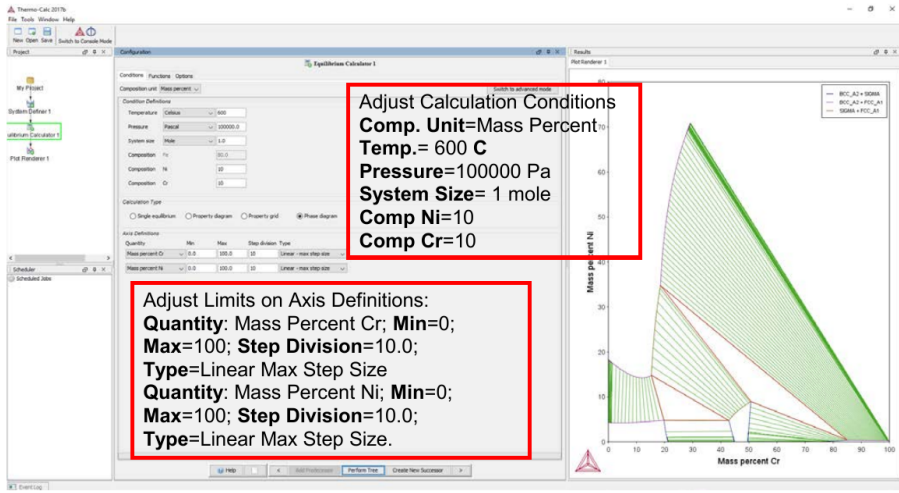
2. Choose the Correct Database and add Elements



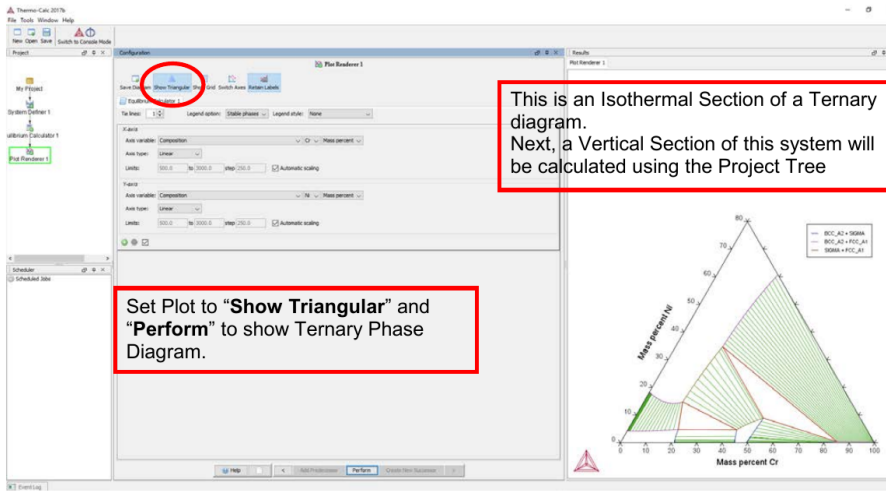
3. Add Phases



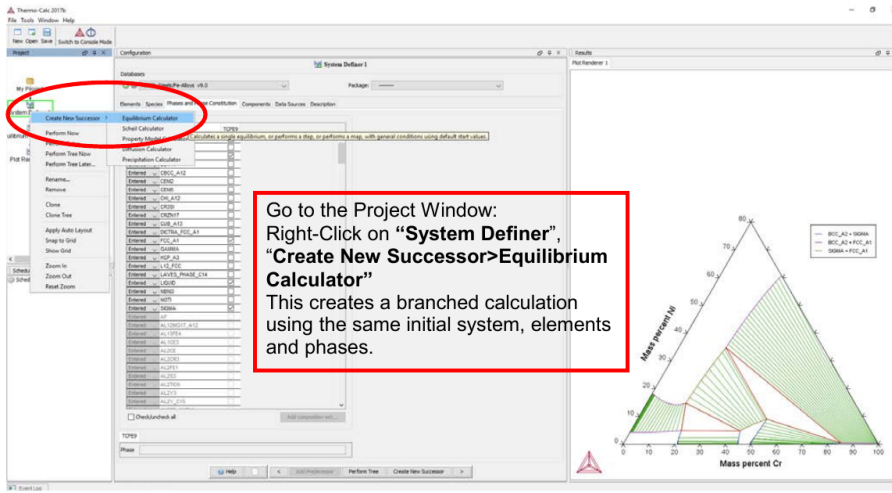
4. Set conditions, then perform calculation.



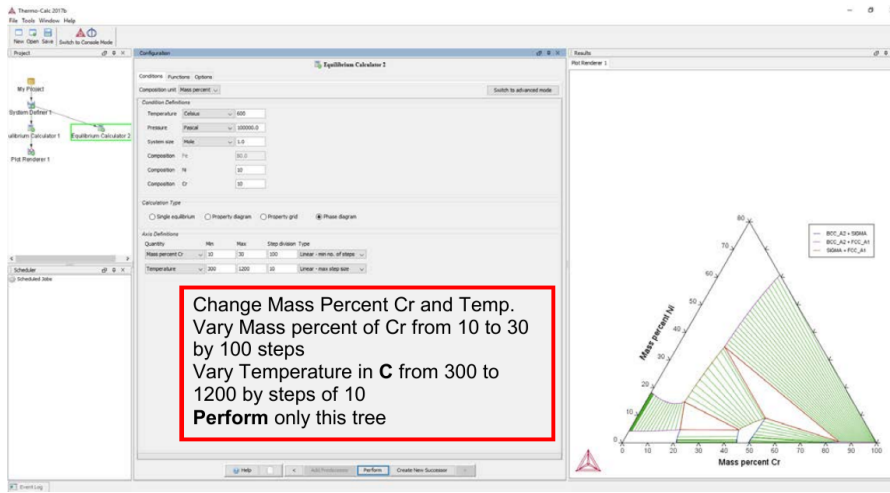
5. Finish the plot as a triangular diagram.



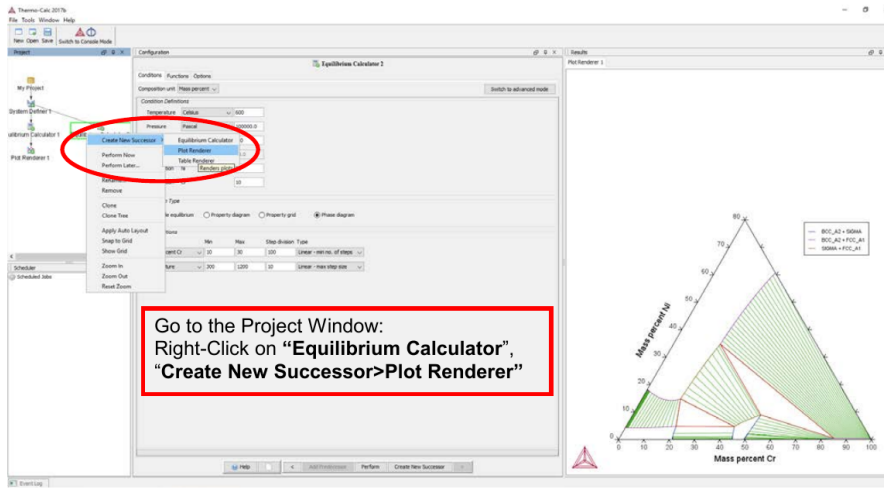
6. Create a new Branch of the Project.



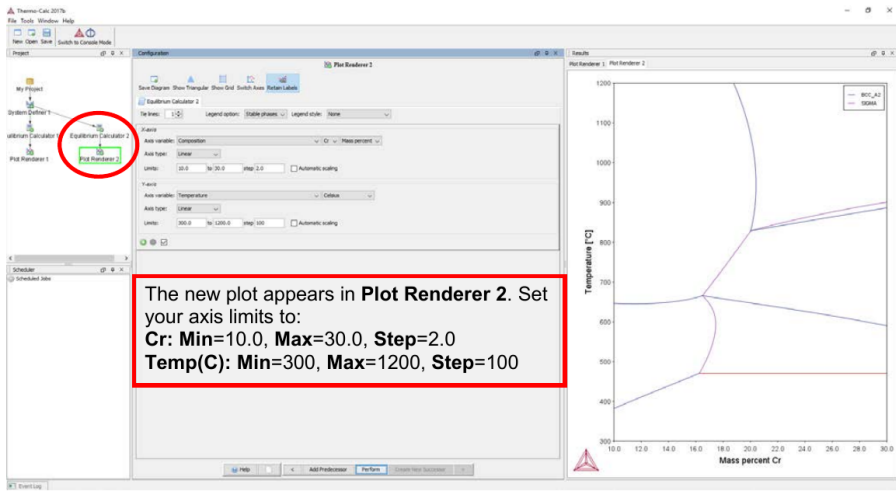
7. Set Conditions and Perform Equilibrium Calculations

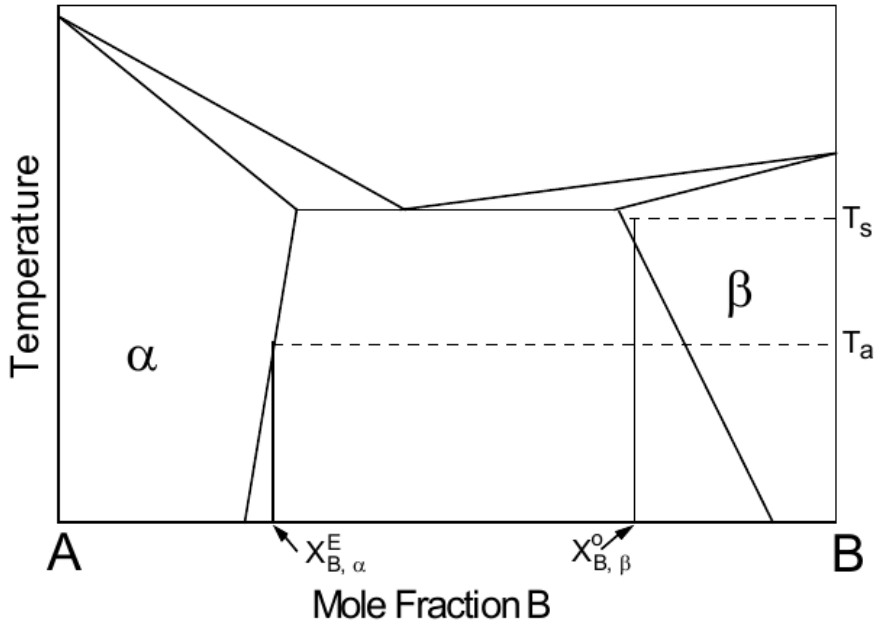


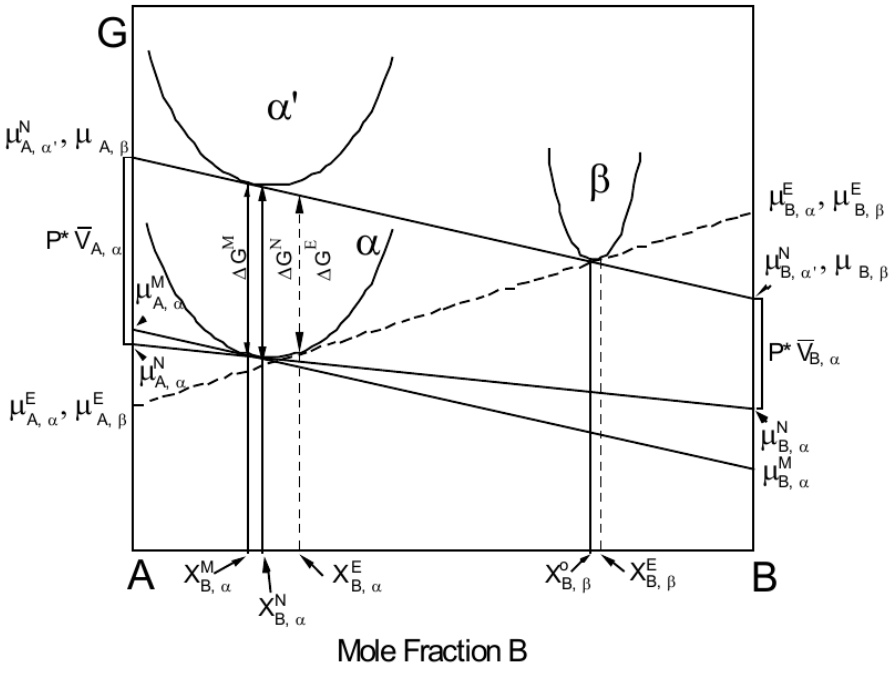
8. Create a new Plot Renderer

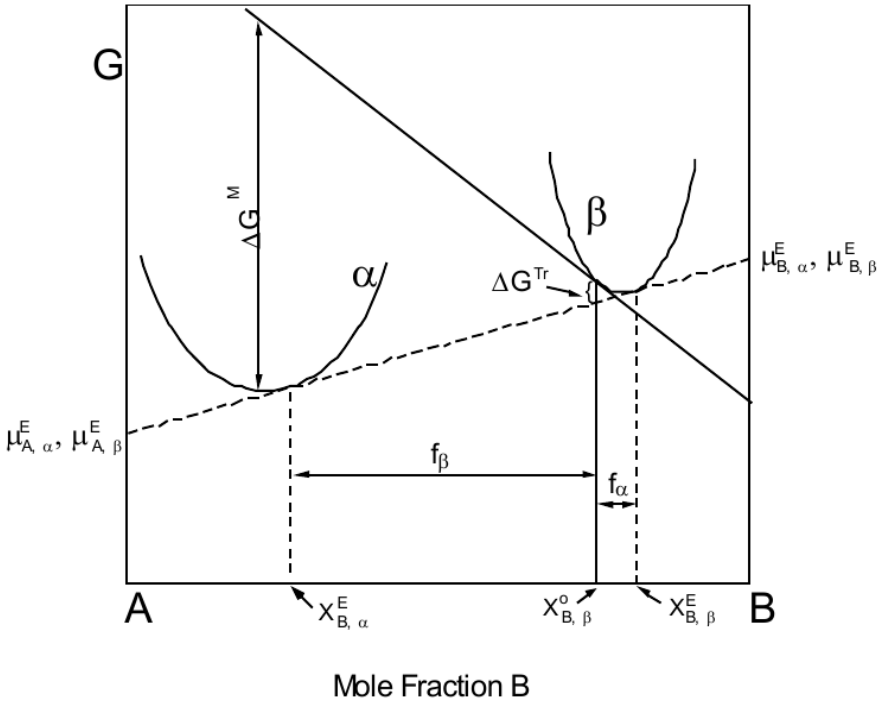


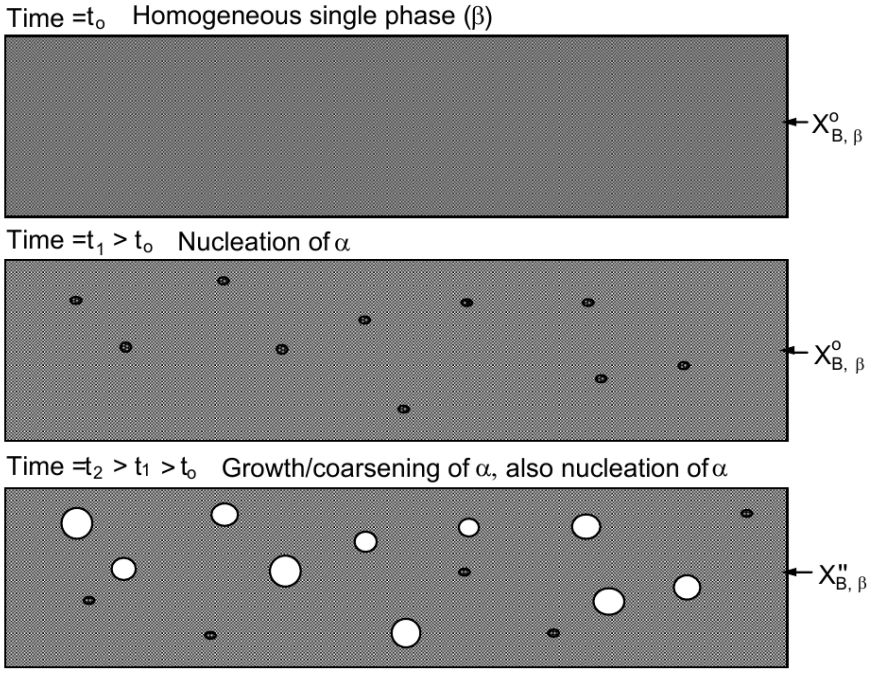
9. Create a new Plot Renderer, Set Plot Axis and Perform




Temperature
α
β
T_s
T_a
A
$X^E_{B,\alpha}$
$X^o_{B,\beta}$
B
Mole Fraction B


G
α'
β
α
$\mu^N_{A,\alpha'}, \mu_{A,\beta}$
$P^* \bar{V}_{A,\alpha}$
ΔG^M
ΔG^N
ΔG^E
$\mu^M_{A,\alpha}$
$\mu^N_{A,\alpha}$
$\mu^E_{A,\alpha}, \mu^E_{A,\beta}$
$\mu^E_{B,\alpha}, \mu^E_{B,\beta}$
$\mu^N_{B,\alpha'}, \mu_{B,\beta}$
$P^* \bar{V}_{B,\alpha}$
$\mu^N_{B,\alpha}$
$\mu^M_{B,\alpha}$
A
$X^M_{B,\alpha}$
$X^N_{B,\alpha}$
$X^E_{B,\alpha}$
$X^o_{B,\beta}$
$X^E_{B,\beta}$
B
Mole Fraction B

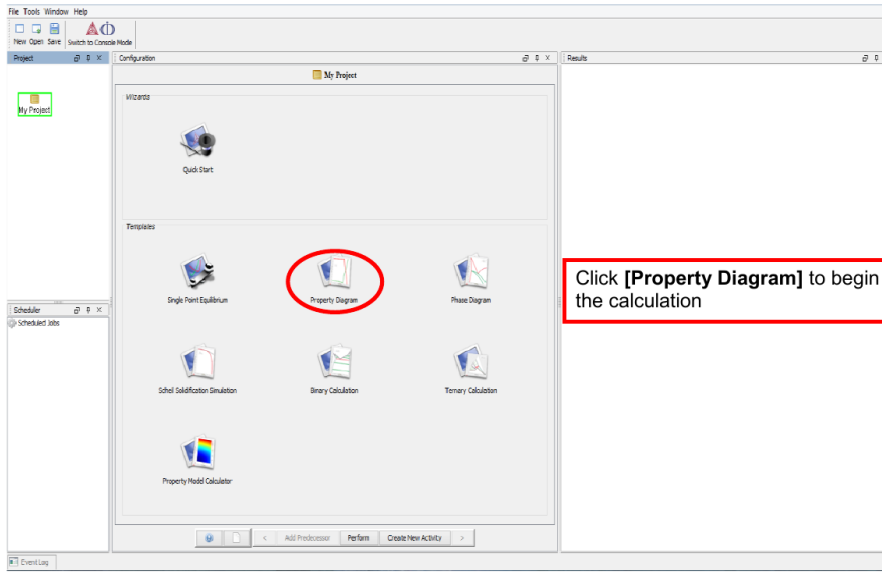

G
ΔG^M
α
β
ΔG^{Tr}
$\mu^E_{B,\alpha}, \mu^E_{B,\beta}$
$\mu^E_{A,\alpha}, \mu^E_{A,\beta}$
f_β
f_α
A
$X^E_{B,\alpha}$
$X^o_{B,\beta}$
$X^E_{B,\beta}$
B
Mole Fraction B



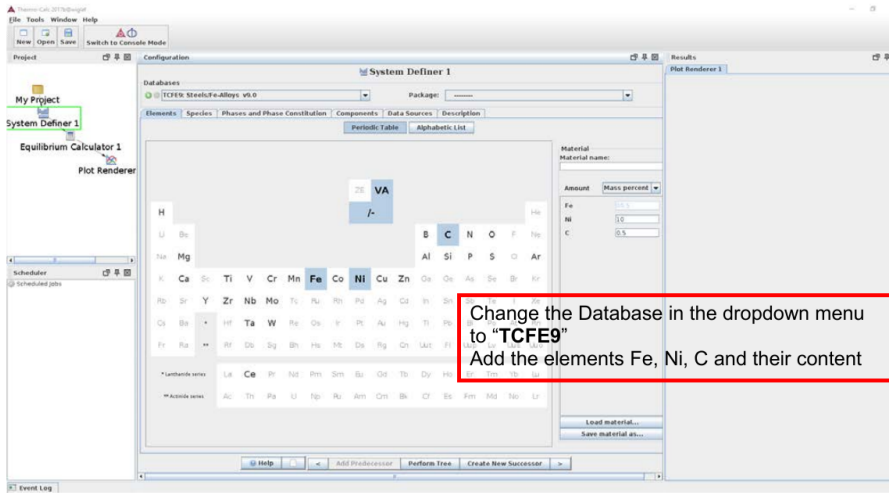
EXAMPLE 5: Composition-Invariant Transformation

There are many examples of phase transformations where the compositions of the parent and product phase are exactly the same. These are called composition-invariant transformations. Examples include massive transformation, martensitic transformation, congruent ordering, congruent melting (or solidification) etc. Then, the driving force for such a transformation (ΔGm) is given by the difference in molar Gibbs energy i.e., $\Delta G_m = G_m(product) - G_m(parent)$. Let us consider a Fe-10Ni-0.5C wt% alloy being cooled continuously from 727 °C to 27 °C. This alloy may undergo a martensitic transformation. For the sake of simplicity, we will approximate martensite as the BCC phase given in ThermoCalc.

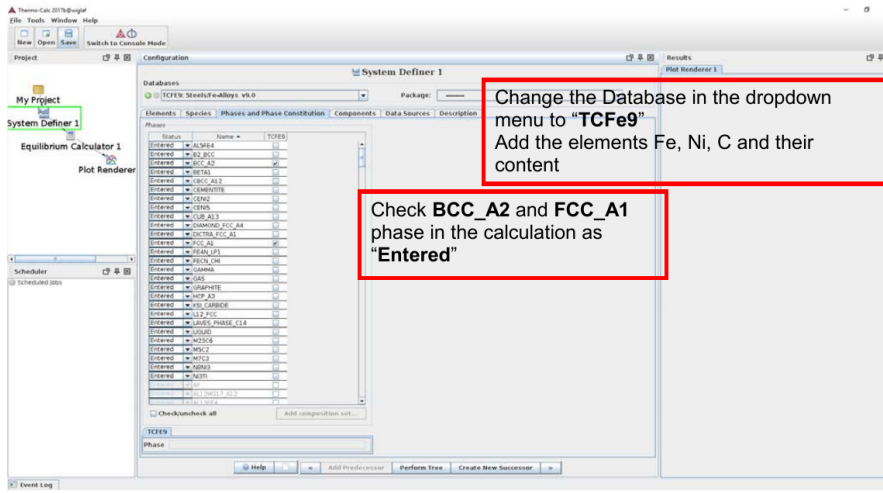
1. Open TC2021b and enter GUI mode. Select 'One Axis Equilibrium'



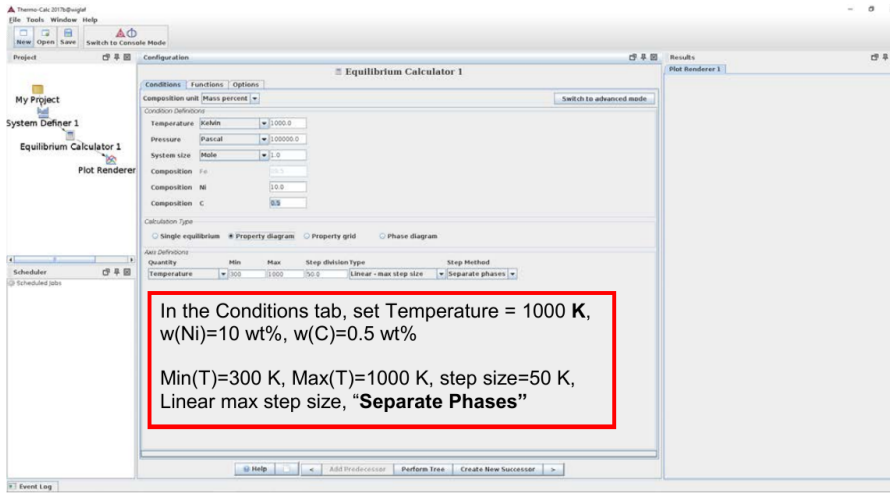
2. Change the database, add the correct elements, go to the Phases tab.



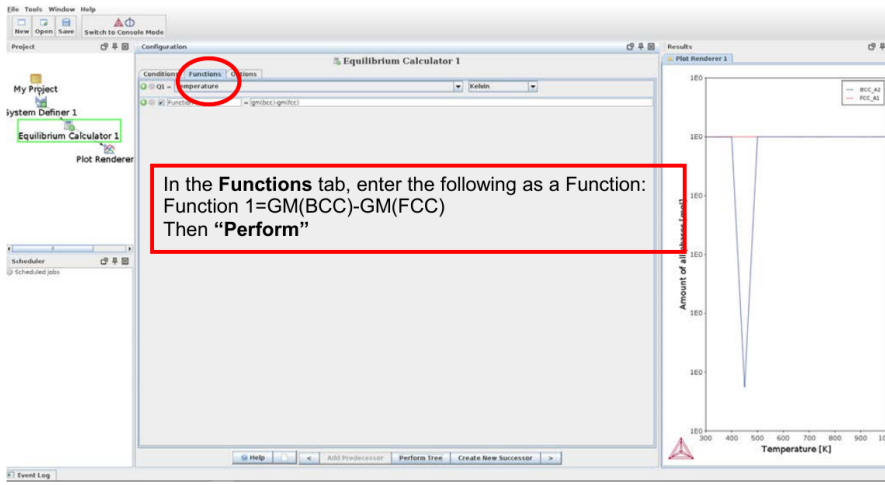
3. Choose Phases



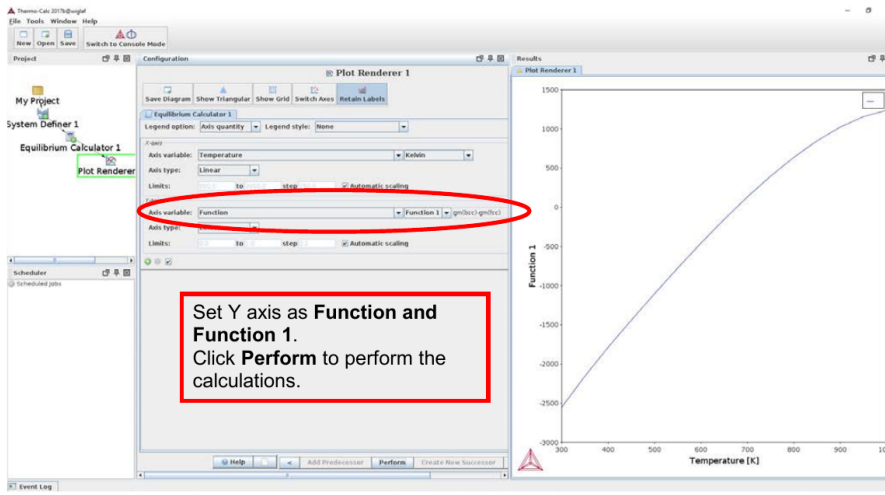
4. Set Conditions (Temperature and Composition).



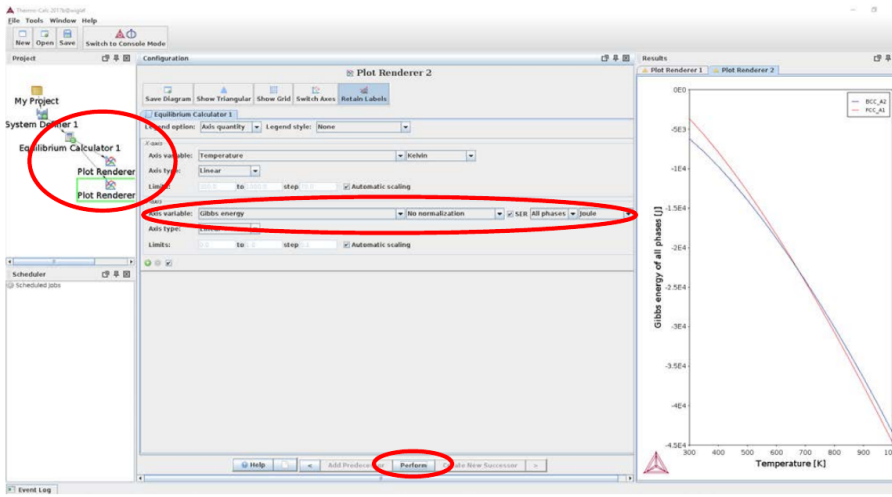
5. Enter Driving Force Functions



6. Adjust Y axis variable & scale



7. Make a New Plot with Gibbs Energy of all phases



- What is the T_0 temperature of the alloy, where T_0 is the temperature where $G_m\,(bcc) = G_m\,(fcc)$ using the plot of Driving Force versus Temperature? Does this correspond to the plot of Gibbs energy versus temperature?
- Assuming that the martensitic transformation starts at a Driving Force of -1000 J/mol, what is the Ms temperature of the above alloy?

Lab 3: DICTRA

Introduction

In this lab you will learn how to simulate the diffusional processes in multicomponent systems using DICTRA (DIffusion Controlled TRAnsformation). DICTRA is a very convenient tool for solving multicomponent diffusion problems with systems having simple geometry, particularly for problems involving a moving boundary. DICTRA combines ThermoCalc with a procedure to solve the diffusion problem and a Newton-Raphson iteration technique to determine the migration rate of the interface and the equilibrium at phase interfaces.

The equation to be solved is Fick's 2nd law of diffusion, which is usually written in the following form:

$$\frac{\partial C_k}{\partial t} = \nabla \left(D_k \nabla C_k \right), \tag{12}$$

where C_k is the concentration of component k, D_k is the diffusion coefficient for component k and ∇ is the gradient operator. It is convenient to separate thermodynamic effects from kinetic effects by introducing, M_k, the diffusive mobility for component k. The diffusion coefficient in this case is:

$$D_k = M_k C_k \frac{\partial \mu_k}{\partial C_k} \tag{13}$$

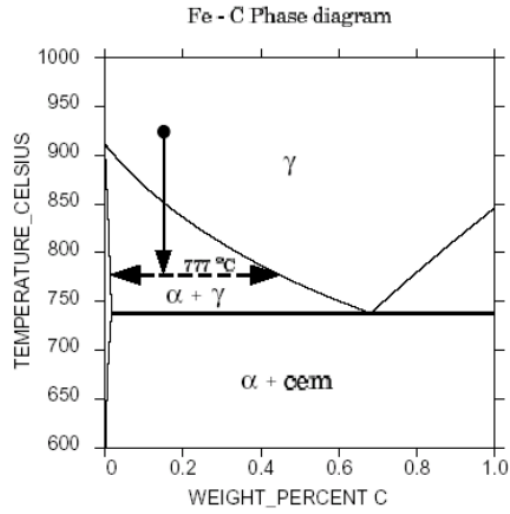
where μ_k is the chemical potential of component k. (See the 316-1 text for a more detailed description). Combination of Eqs. 12 and 13 gives:

$$\frac{\partial C_k}{\partial t} = \nabla \left(C_k M_k \nabla \mu_k \right), \tag{14}$$

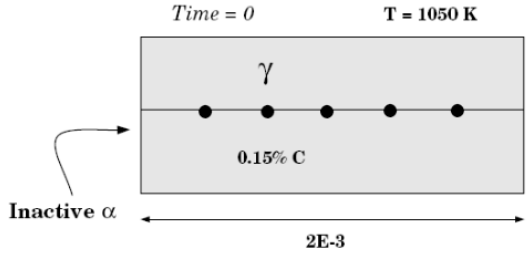
The diffusion database holds the mobility terms and the chemical potentials are extracted from the thermodynamic database. DICTRA solves Eq. 14 at every grid point using Thermo-Calc to calculate the composition-dependent chemical potentials. (The numerical simulation is basically the same sort of thing that COMSOL does, but DICTRA interfaces directly with the thermodynamic databases embedded in Thermo-Calc).

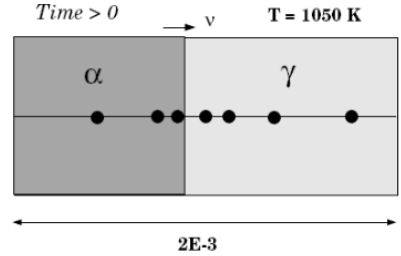
Example: γ to α transformation in a binary Fe-C alloy.

This example deals with the kinetics of phase transformation from austenite (γ-fcc) to ferrite (α-bcc) in a binary Fe-C alloy upon cooling and then maintaining a fixed temperature. We will start the simulation at a high temperature at 1173 K (900 °C) and we assume a gradual cooling down to 1050 K (777 °C) at a cooling rate of 10 K/minute. When we reach 1050 K we keep the temperature constant and thus have an isothermal transformation. The composition of the alloy is Fe – 0.15wt%C:

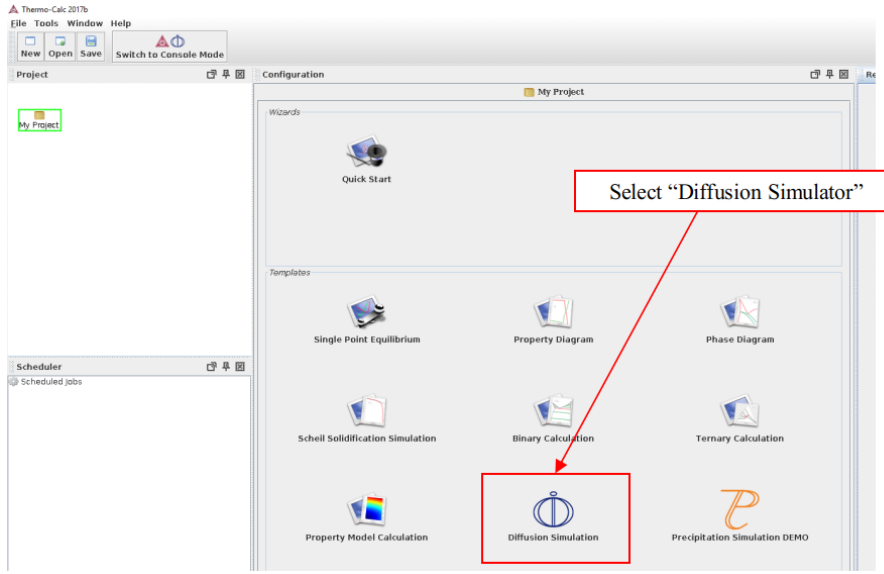

Fe - C Phase diagram
TEMPERATURE_CELSIUS
WEIGHT_PERCENT C
1000
950
900
850
800
750
700
650
600
0
0.2
0.4
0.6
0.8
1.0
γ
77 °C
α + γ
α + cem

(Inactive α)

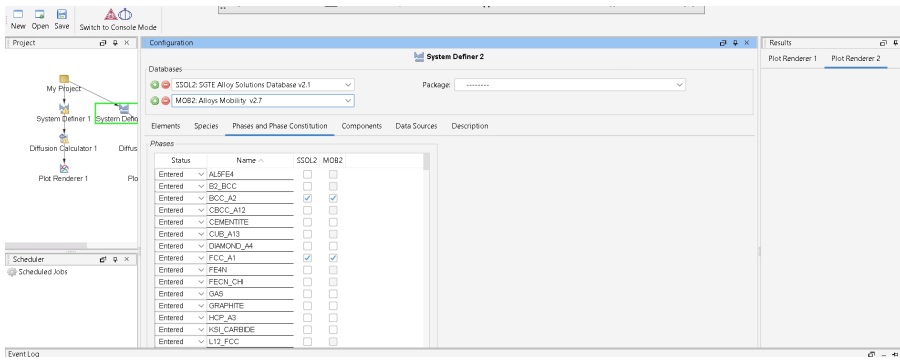

Time = 0
T = 1050 K
γ
0.15% C
Inactive α
2E-3

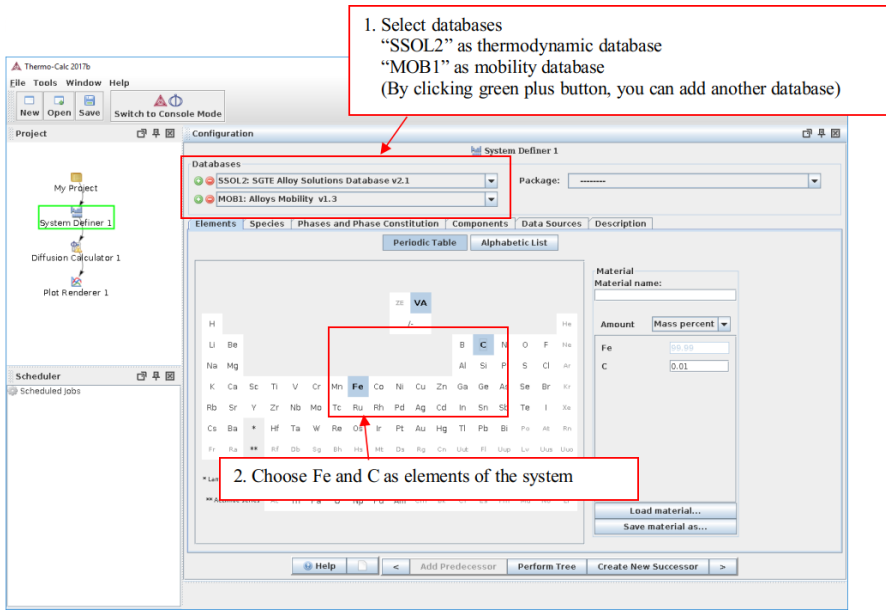

Time > 0
v
T = 1050 K
α
γ
2E-3

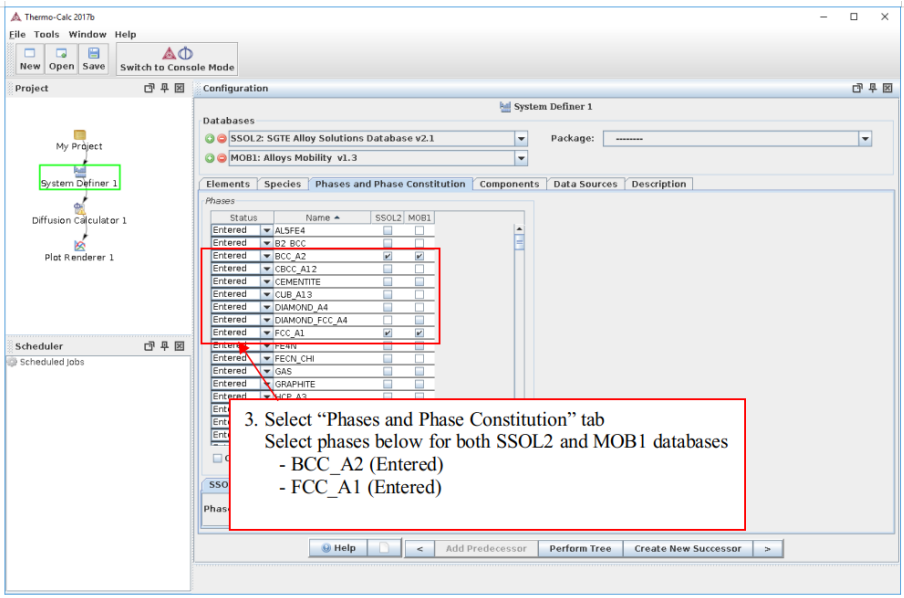
Step 1: Open Thermo-Calc 2021b and select "Diffusion Simulation"



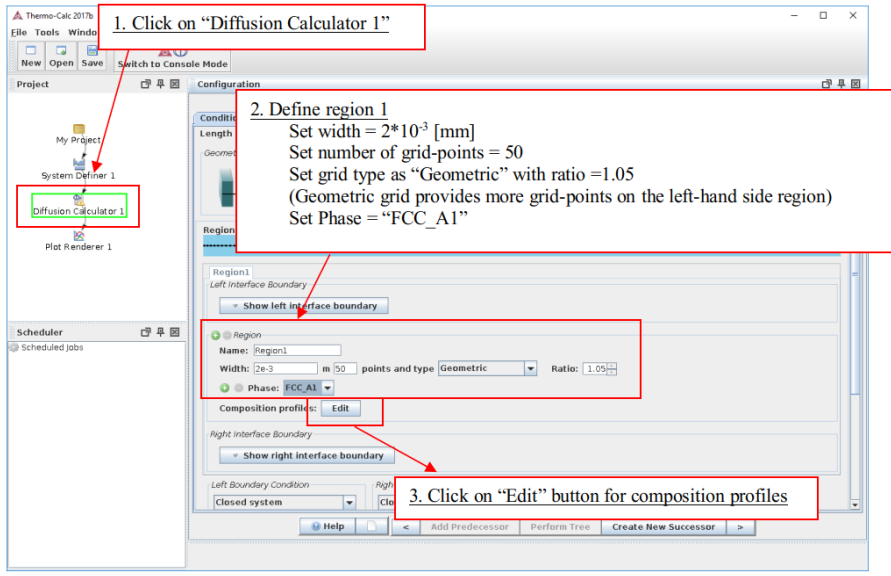
Step 2: Define The system: 1) Check "SSOL2" as the thermodynamic database, and "MOB1" as the mobility database.

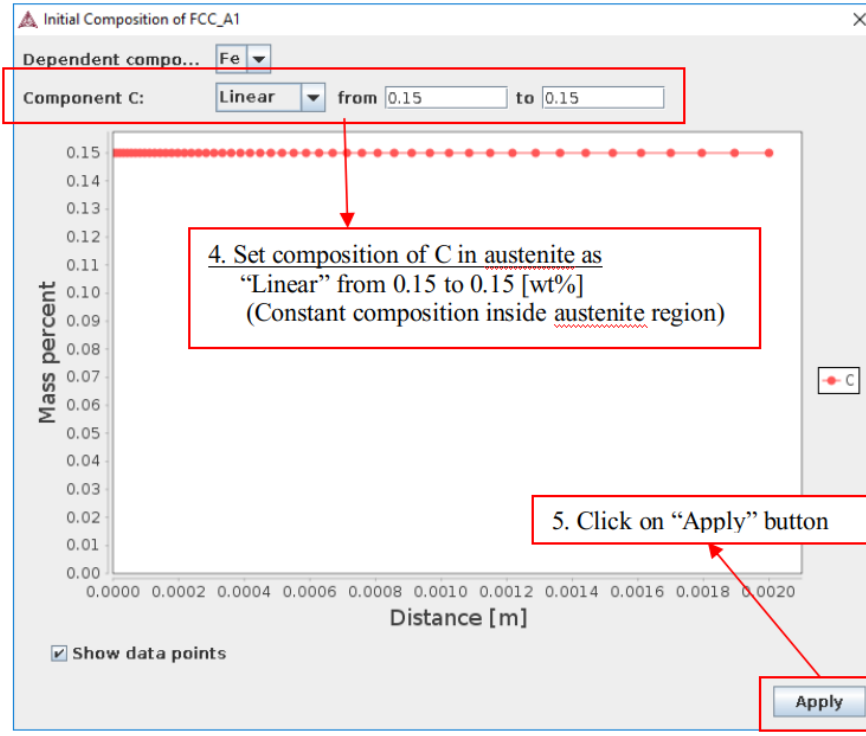


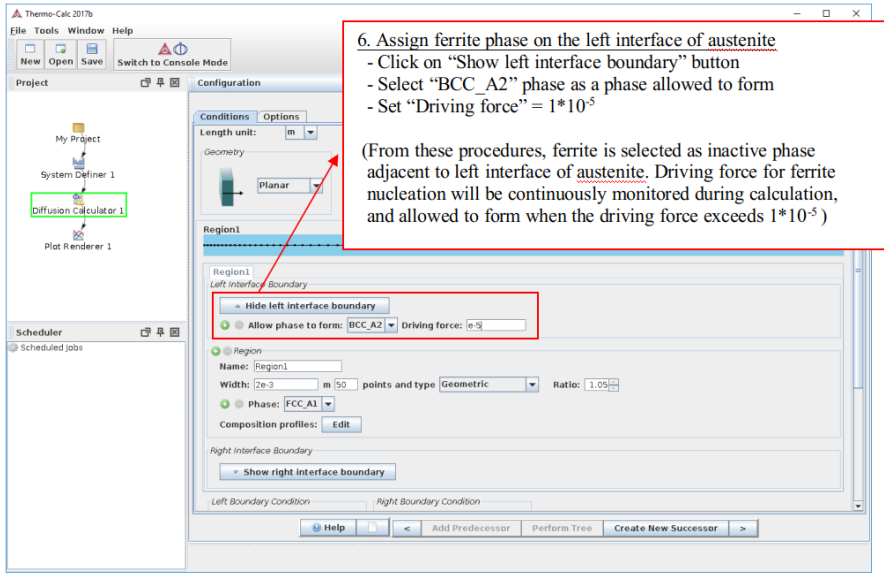

1. Select databases
"SSOL2" as thermodynamic database
"MOB1" as mobility database
(By clicking green plus button, you can add another database)
2. Choose Fe and C as elements of the system

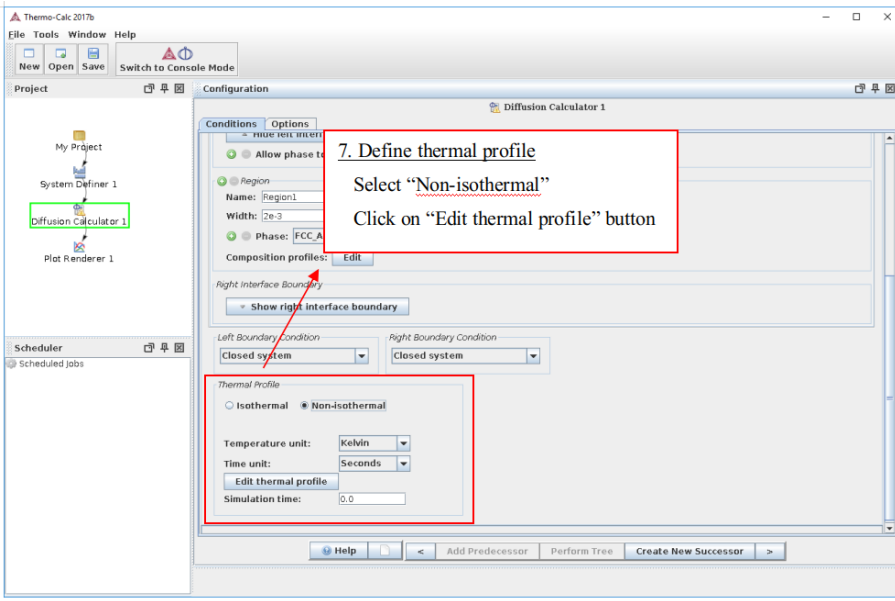

3. Select "Phases and Phase Constitution" tab
Select phases below for both SSOL2 and MOB1 databases
- BCC_A2 (Entered)
- FCC_A1 (Entered)

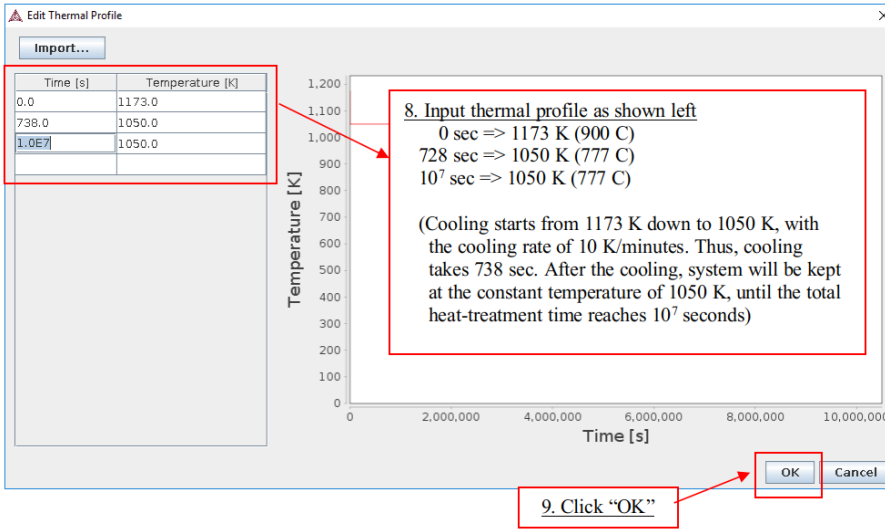
Define Calculation Conditions

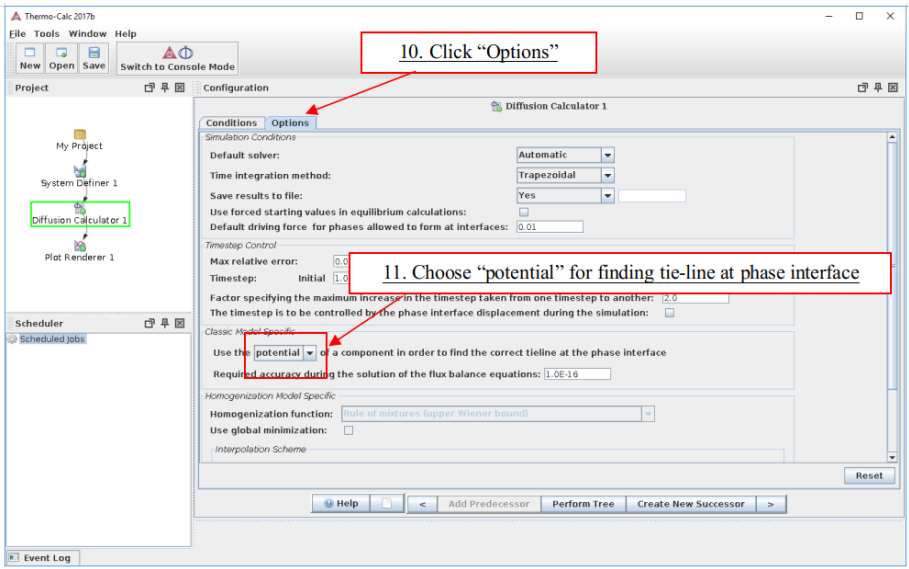




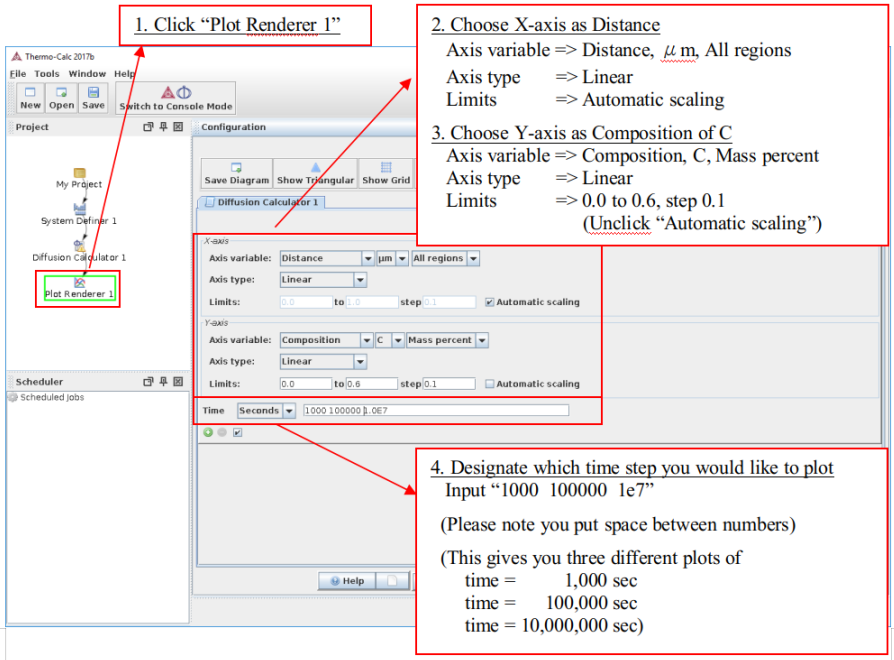

6. Assign ferrite phase on the left interface of austenite
- Click on "Show left interface boundary" button
- Select "BCC_A2" phase as a phase allowed to form
- Set "Driving force" = 1*10-5
(From these procedures, ferrite is selected as inactive phase adjacent to left interface of austenite. Driving force for ferrite nucleation will be continuously monitored during calculation, and allowed to form when the driving force exceeds 1*10-5)
Thermo-Calc 2017b
File Tools Window Help
New Open Save
Switch to Console Mode
Project
Configuration
My Project
System Definer 1
Diffusion Calculator 1
Plot Renderer 1
Scheduler
Scheduled Jobs
Conditions Options
Length unit: m
Geometry
Planar
Region1
Left Interface Boundary
Hide left interface boundary
Allow phase to form: BCC_A2 Driving force: 1e-5
Region
Name: Region1
Width: 2e-3 m 50 points and type Geometric Ratio: 1.05
Phase: FCC_A1
Composition profiles: Edit
Right Interface Boundary
Show right interface boundary
Left Boundary Condition
Right Boundary Condition
Help
Add Predecessor
Perform Tree
Create New Successor


7. Define thermal profile
Select "Non-isothermal"
Click on "Edit thermal profile" button
Thermo-Calc 2017b
File Tools Window Help
New Open Save
Switch to Console Mode
Project
Configuration
Diffusion Calculator 1
My Project
System Definer 1
Diffusion Calculator 1
Plot Renderer 1
Scheduler
Scheduled Jobs
Conditions Options
Region
Name: Region1
Width: 2e-3
Phase:
Composition profiles: Edit
Right Interface Boundary
Show right interface boundary
Left Boundary Condition
Closed system
Right Boundary Condition
Closed system
Thermal Profile
Isothermal
Non-isothermal
Temperature unit: Kelvin
Time unit: Seconds
Edit thermal profile
Simulation time: 0.0
Help
Add Predecessor
Perform Tree
Create New Successor

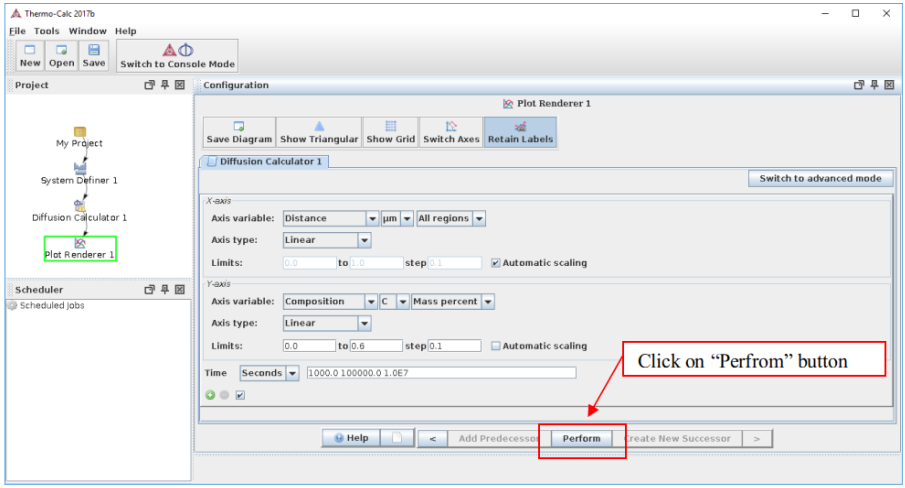

Edit Thermal Profile
Import...
Time [s]
Temperature [K]
0.0
1173.0
738.0
1050.0
1.0E7
1050.0
Temperature [K]
Time [s]
8. Input thermal profile as shown left
0 sec => 1173 K (900 C)
728 sec => 1050 K (777 C)
10^7 sec => 1050 K (777 C)
(Cooling starts from 1173 K down to 1050 K, with the cooling rate of 10 K/minutes. Thus, cooling takes 738 sec. After the cooling, system will be kept at the constant temperature of 1050 K, until the total heat-treatment time reaches 10^7 seconds)
OK
Cancel
9. Click "OK"


Thermo-Calc 2017b
File Tools Window Help
New Open Save
Switch to Console Mode
10. Click "Options"
Project
Configuration
Diffusion Calculator 1
My Project
System Definer 1
Diffusion Calculator 1
Plot Renderer 1
Conditions
Options
Simulation Conditions
Default solver:
Automatic
Time integration method:
Trapezoidal
Save results to file:
Yes
Use forced starting values in equilibrium calculations:
Default driving force for phases allowed to form at interfaces:
0.01
Timestep Control
Max relative error:
Timestep:
Initial
11. Choose "potential" for finding tie-line at phase interface
Factor specifying the maximum increase in the timestep taken from one timestep to another:
2.0
The timestep is to be controlled by the phase interface displacement during the simulation:
Classic Model Specific
Use the potential of a component in order to find the correct tieline at the phase interface
Required accuracy during the solution of the flux balance equations:
1.0E-16
Homogenization Model Specific
Homogenization function:
Rule of mixtures (upper Wiener bound)
Use global minimization:
Interpolation Scheme
Reset
Scheduler
Scheduled Jobs
Help
Add Predecessor
Perform Tree
Create New Successor
Event Log

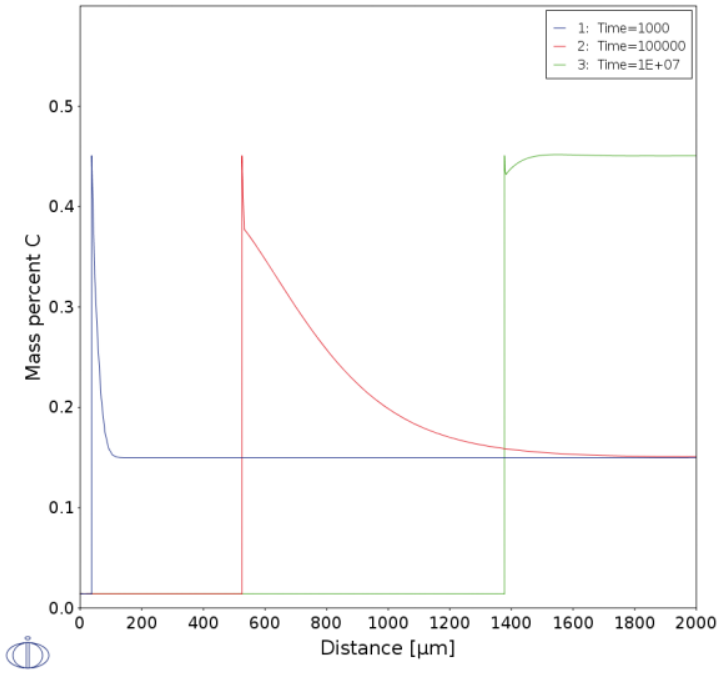
Step 4: Define Plot Conditions



Step 5: Execute Calculation



Step 6: Interpret the Result



As the deliverable for this lab, please upload to Canvas a screenshot of the DICTRA interface that includes your version of the plot with the carbon concentration profiles.

Lab 4: PrecipiCalc/TC-PRISMA

PrecipiCalc Overview

What is PrecipiCalc?

- Sophisticated software for calculating the precipitation kinetics of second phase transformations.
- Developed by Questek Innovations LLC.
- Platform: UNIX, MS Windows.

What PrecipiCalc does?

- Realistic and mechanistic modeling of nucleation, growth and coarsening without resorting to ad hoc treatments
- Relies on DICTRA (Diffusion Controlled TRAnsformation) to perform fundamental thermodynamics and mobility calculations

Applications

- Materials processing & Materials design

PrecipiCalc Architecture

Layered Architecture Pattern.

Five layers where each layer may provide services to all the layers above

- Layer I: PrecipiCalc class, the top layer – calculating core particle size distribution evolution
- Layer II: pcNucleation, pcTemperature, pcEnd – nucleation model, temperature profile and termination model
- Layer III: pcGrowth – growth model based on multi-component thermodynamics and kinetics
- Layer IV: pcLP, pcSurfEng – lattice parameter (molar volume) and surface energy
- Layer V: pcStore class, the bottom layer – storage of particle size distribution and its associated quantities (e.g. volume fraction, mean size)

TC-PRISMA

The Precipitation module (TC-PRISMA) is an add-on module in Thermo-Calc which treats concurrent nucleation, growth/dissolution and coarsening under arbitrary heat treatment conditions in multi-component and multi-phase systems using Langer-Schwartz theory and the Kampmann-Wagner numerical approach. The Precipitation module (TC-PRISMA) extends the functionality available through Thermo-Calc and the Diffusion module (DICTRA) and can be used for calculations of:

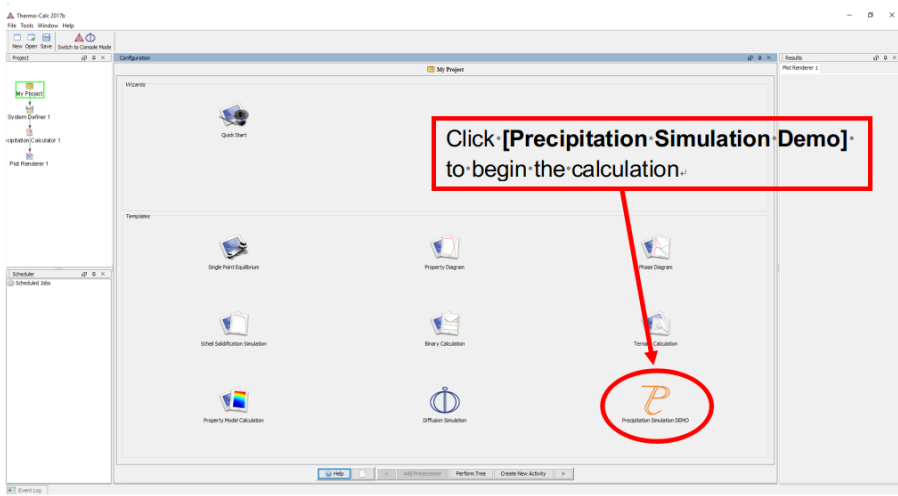
- Concurrent nucleation, growth/dissolution and coarsening of precipitates
- Temporal evolution of particle size distribution
- Average particle radius and number density
- Volume fraction and composition of precipitate
- Nucleation rate and coarsening rate
- Isothermal transformation/Time-Temperature-Transformation (TTT) diagrams
- Continuous-Cooling-Transformation (CCT) diagrams
- Estimation of multi-component interfacial energy

Lab Deliverables for each student: Screenshot of final result for each of the 3 examples.

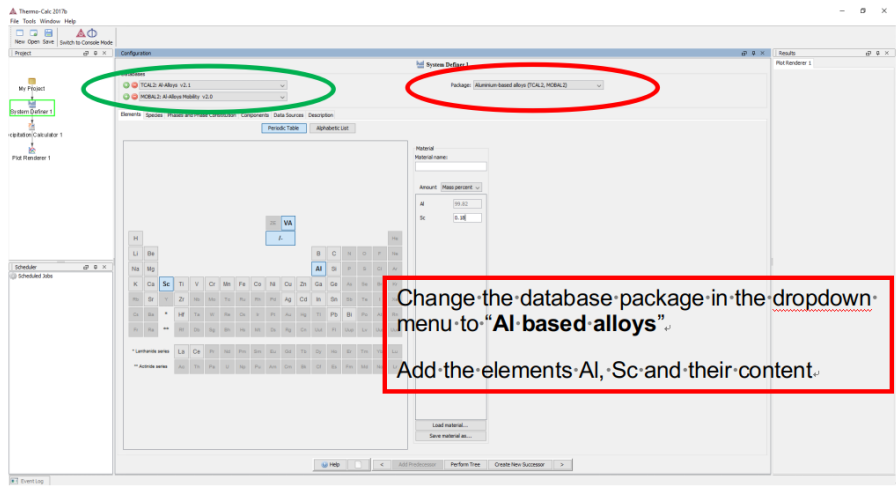
Example 1. Isothermal Precipitation of Al_3Sc in Al-0.18Sc (wt%) binary alloy

This example simulates the kinetics of precipitation of Al_3Sc from an FCC_A1 solution phase.

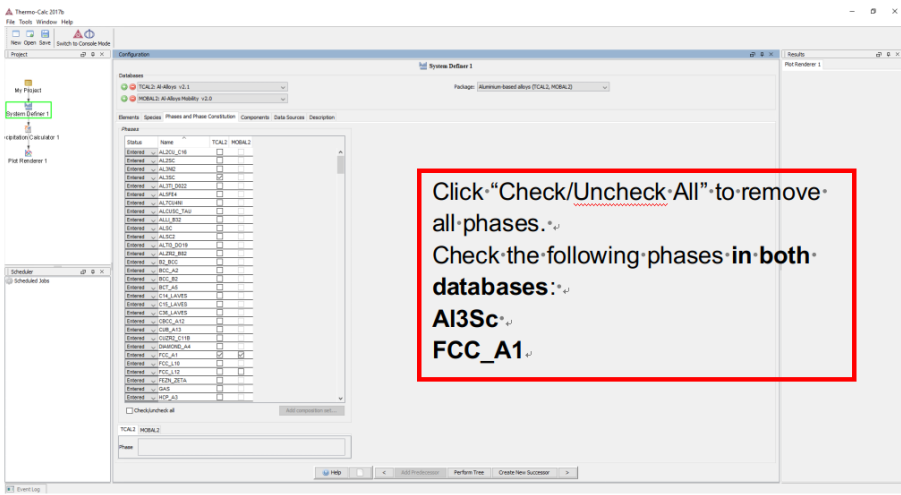
Step 1: Open TC2021b and enter GUI. Select 'TC-PRISMA'



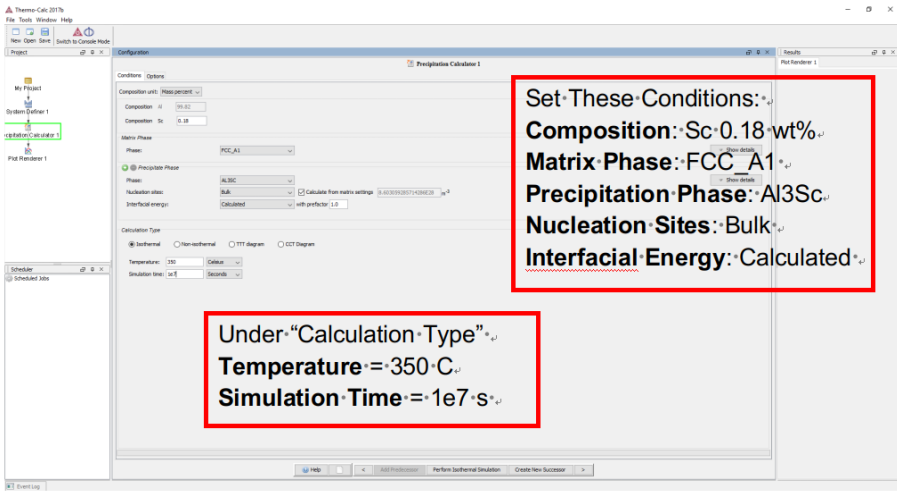
Step 2: Pick Database and Elements in System



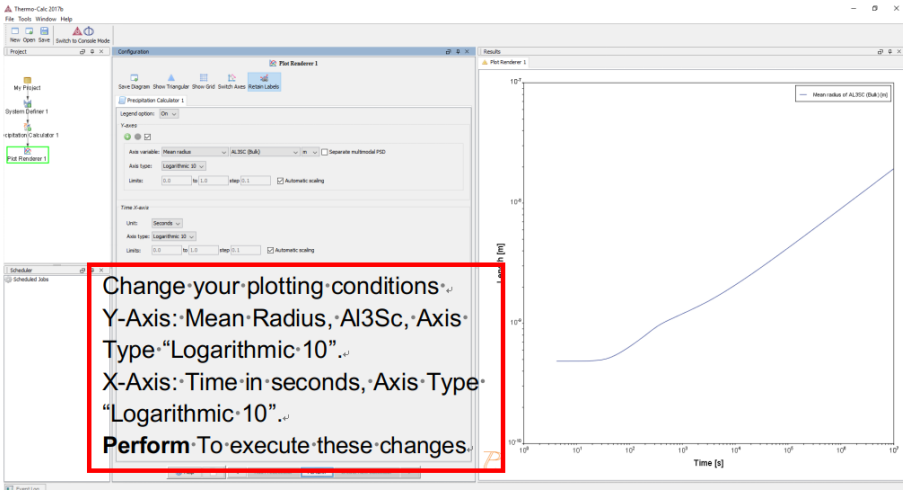
Step 3: Identify Phases in System



Step 4: Set Simulation Conditions. Then Perform calculation. (The calculation would take a few minutes).

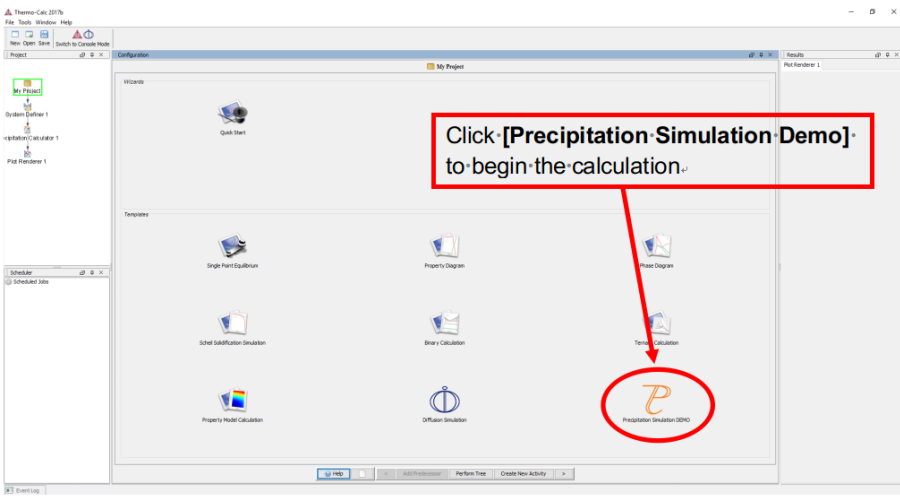


Step 5: Plot Renderer Results

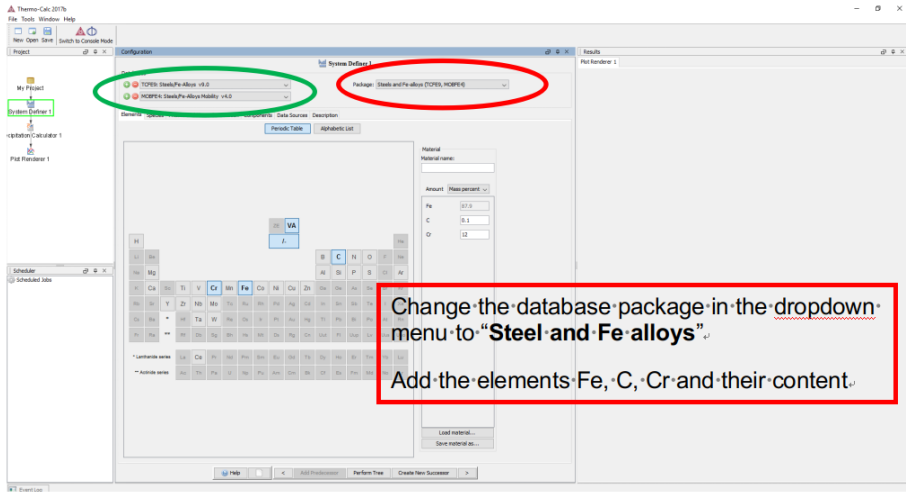


Example 2. Stable and Metastable Carbides in Fe-0.1C-12Cr (wt%) Steel - TTT Diagram

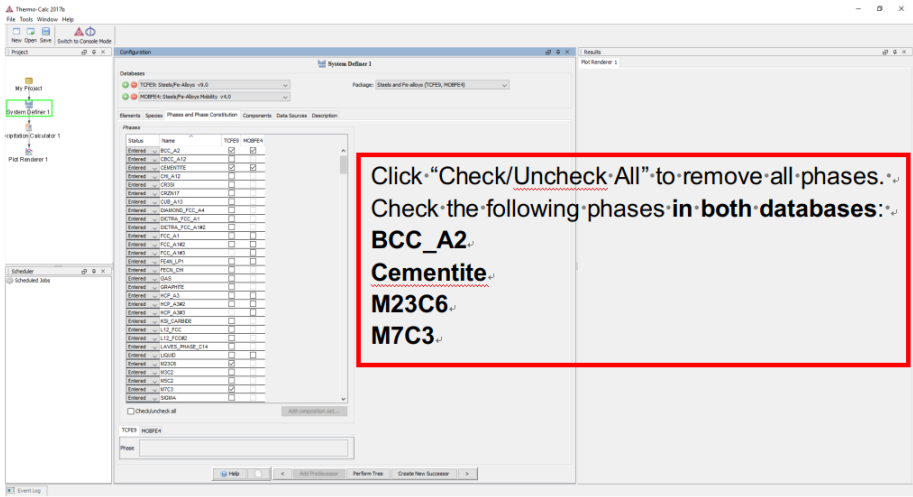
Step 1: Open TC2021b and enter GUI. Select 'TC-PRISMA'



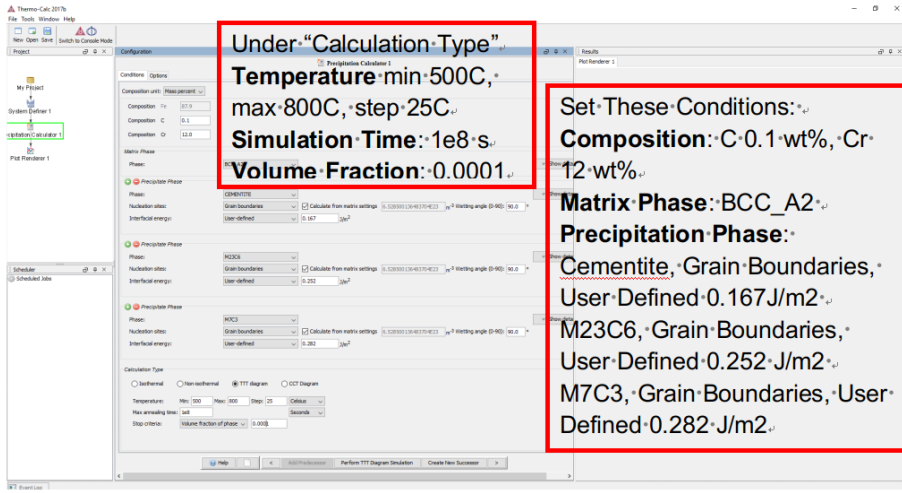
Step 2: Pick Database and Elements in System



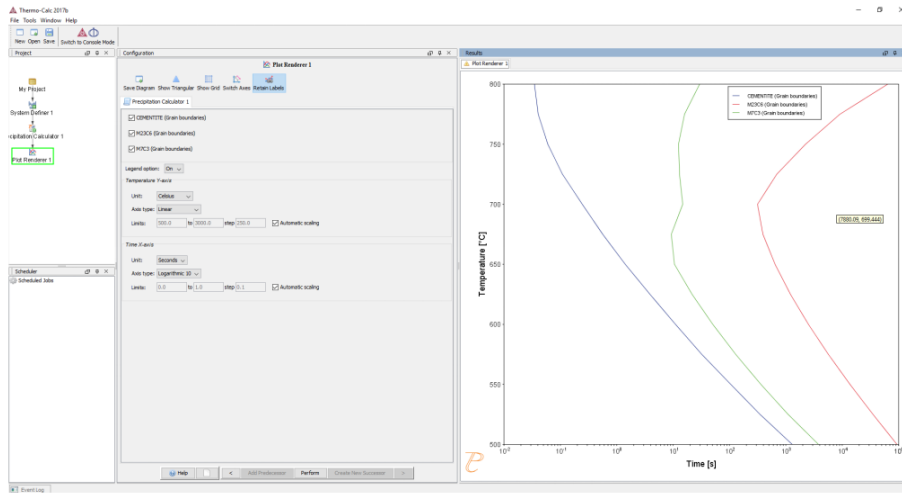
Step 3: Identify Phases in System



Step 4: Set Simulation Conditions for TTT diagram. Then Perform calculation. (The calculation will take a few minutes.)



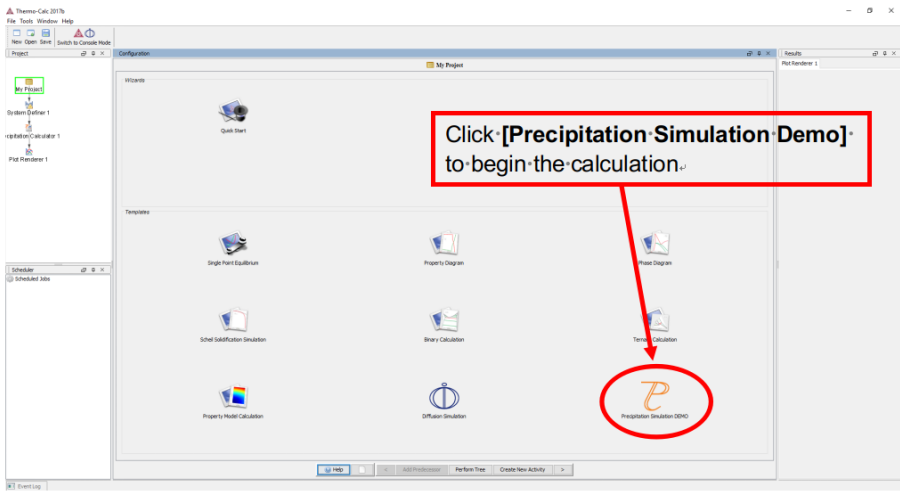
Step 5: Plot Renderer Results



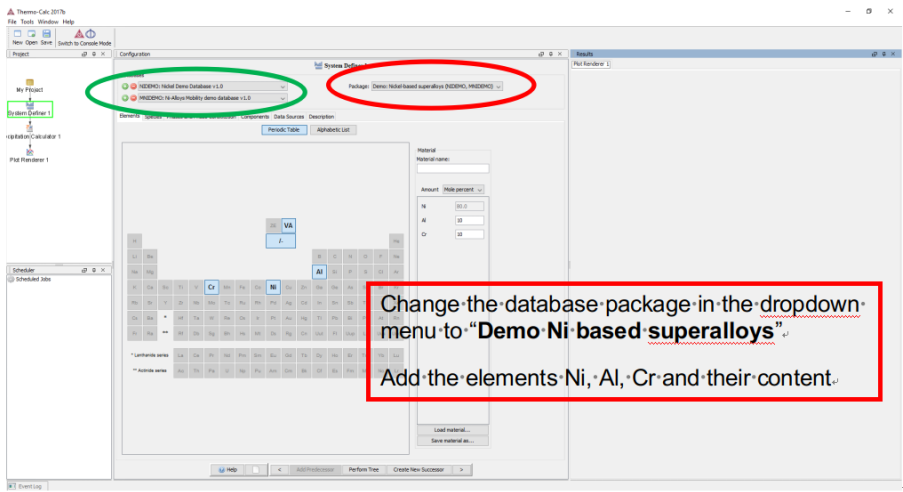
Example 3. Cooling Rate Diagram of $\gamma - \gamma'$ Ni-10Al-10Cr (at%) superalloy – CCT diagram

In this example, a CCT diagram for a Ni-10Al-10Cr $\gamma - \gamma'$ alloy is calculated and plotted with superimposition of the cooling rate values.

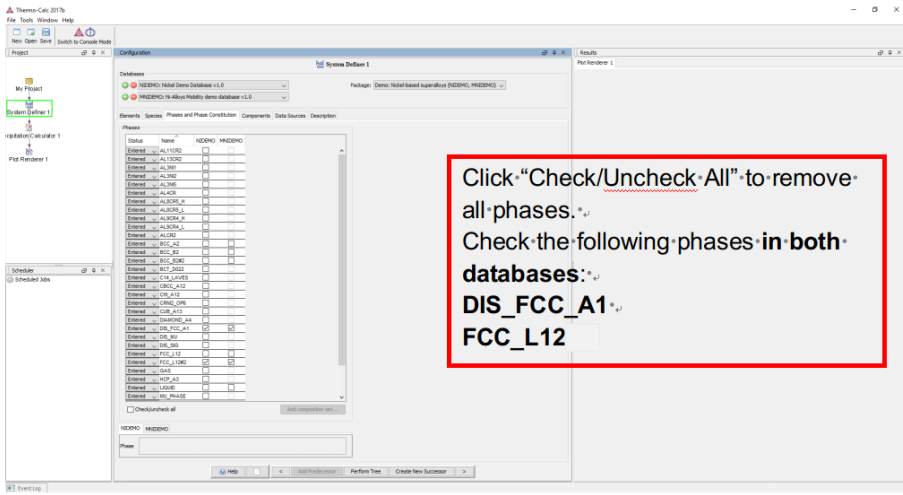
Step 1: Open TC2021b and enter GUI. Select 'TC-PRISMA'



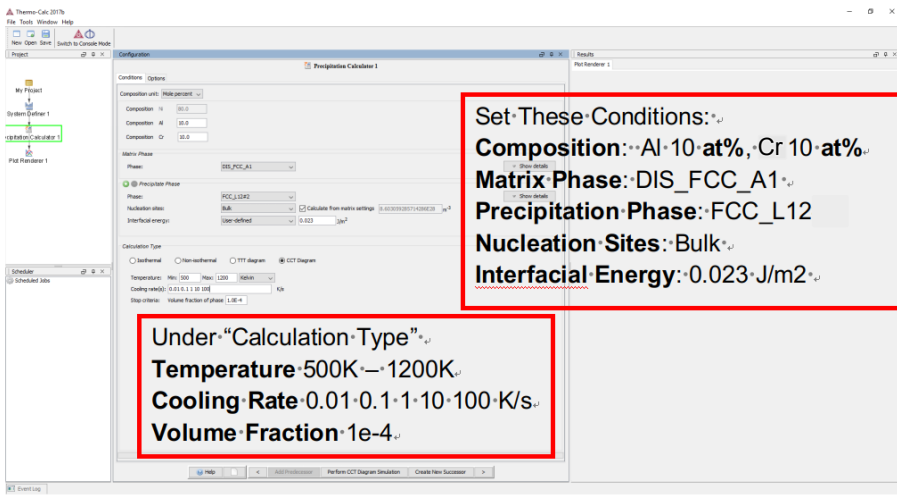
Step 2: Pick Database and Elements in System



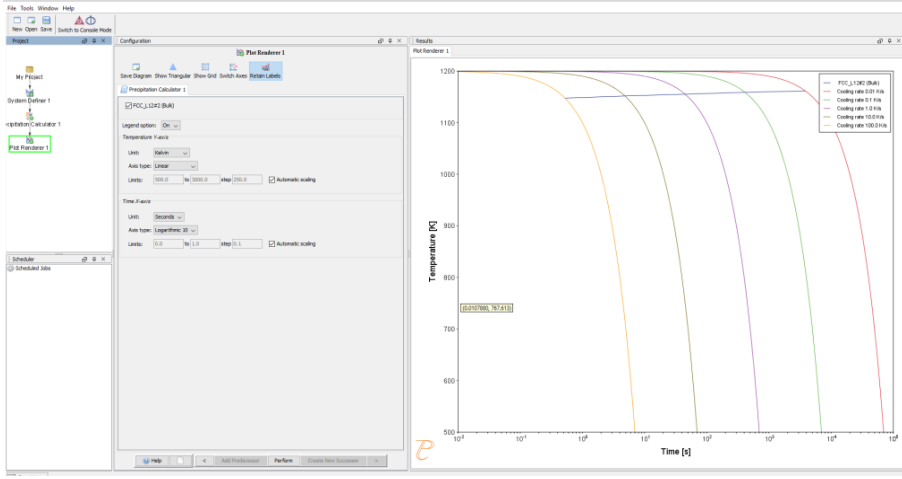
Step 3: Identify Phases in System

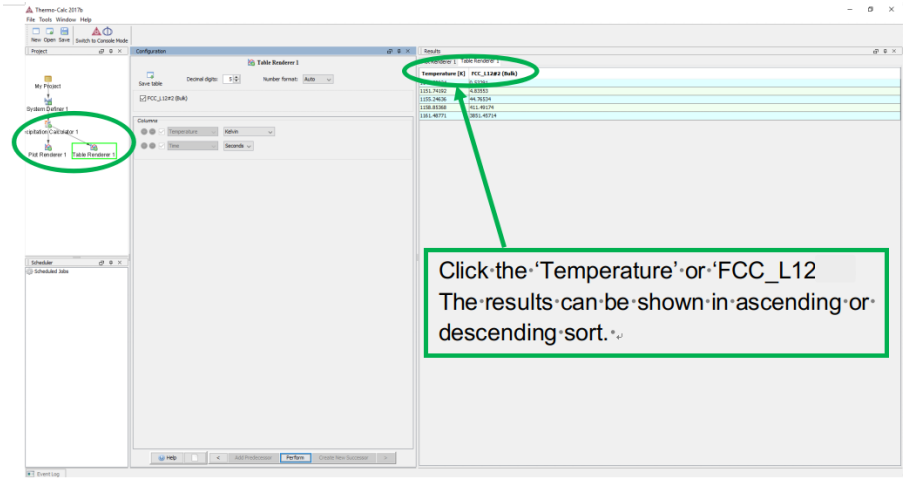


Step 4: Set Simulation Conditions for CCT diagram. Then Perform calculation. The calculation would take a few minutes.



Step 5: Plot/Table Renderer Results


Temperature [K]
Time [s]


Click the 'Temperature' or 'FCC_L12
The results can be shown in ascending or
descending sort.