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1 Syllabus

Syllabus

Updated November 27, 2024

Course Information

Northwestern Syllabus Standards

This course follows the Northwestern University Syllabus Standards. Students are responsible for familiarizing themselves with this information.

Lecture: Tues/Thurs 2:00-3:20 pm AM, Tech C115 (Bodeen Lab)

Instructors:

Prof. K. Shull (k-shull@northwestern.edu)

Teaching Assistants:

Broderick Lewis (broderick.lewis@northwestern.edu)

Online Text: (with syllabus, labs, homeworks)
http://msecore.northwestern.edu/390/390text.pdf

Lecture Slides:

http://msecore.northwestern.edu/390/390slides.pdf

Syllabus:

http://msecore.northwestern.edu/390/390syllabus.pdf

Required Software:

1. Ansys Granta EduPack 2021 R2. There are three ways to access this:
   (a) available on the computers in the teaching lab and in Bodeen (Tech C115).
   (b) If you have a Windows computer, it can also be installed on your own computer by following these instructions:
      i. Download the software here.
      ii. Extract the zipped file locally.
      iii. Run the edupack_setup.2021_R2.exe file.
      iv. When the license information is requested, simply point it towards the server at rho.mcc.northwestern.edu. Leave the port the same (1055).
   (c) A system-independent way to access the Grant Software is available via NUWorkspace. This will work for Windows, Mac and Linux machines. Just click on the link below an then Navigate to the software you want (in this case Granta EduPack):

      https://northwestern.apporto.com/

2. Thermocalc/DICTRA/PrecipiCalc: Available on Bodeen and MSE Teaching Lab computers. The software can also be accessed remotely by setting through the McCormick Virtual Computer lab. Details on how to access it are available at the following link: https://www.mccormick.northwestern.edu/it-resources/labs/virtual-computer-labs.html

Other Resources:

https://www.lucidchart.com: Useful site for building system design charts. A free account should allow you to do everything you need for 390.

https://www.overleaf.com/: Software for producing written report in a standardized format.

http://msecore.northwestern.edu/390/standards_OSU.pdf: Slide deck from Ohio State on the use of professional standards.)

Prof. Office Hours: Send me an email or chat during class and we'll set something up.

TA Office Hours: TBD.

Prerequisites: MSE 314/315/316/331 or equivalent.

Grading and Rubrics:

5%: Lab tutorials

15%: Homeworks

20%: Project Report

- ◇ 10% Clearly presented design chart, linked to the overall goals of the project
- ◇ 10% Quantitative performance metrics, distinct from properties. Use at least one professional standard to define some aspect of your performance metric.
- ◇ 10% Quantitative property targets with well-defined basis for choosing these values
- ◇ 10% Use of the EduPack Materials Selection Software in some meaningful way for your project, with rationalizations for quantitative property targets. Include enough information so that the process could be repeated by someone else.
- ◇ 10% Introduction of your design strategy, describing the focus of your project and how it will relate to some specific aspect of your design chart
- ◇ 20% Presentation of results (see analysis, modeling and experimentation section)
- ◇ 10% Specific design recommendation based on your results.
- ◇ 20% Appropriate referencing (I expect that about 20 references will be appropriate in most cases)

20%: Project Presentation:

- ◇ 10% Appropriate timing: about 20 minutes (not more, a minute or two less okay to leave time for questions).
- ◇ 10% Clear use of slides (fonts big enough to see, etc.)
- ◇ 10% Audibility: This is pretty obvious, but we need to be able to hear you well. I'm not sure our current room is the best for this particular aspect of things, so we might move the presentations to another room
- ◇ Content: You don't need to talk about everything you did, but someone hearing the talk should understand the following:
  - 10% Why your project matters - this generally comes from your introductory slides, where the topic is introduced

  - 10% One slide should be labeled 'Standards', and should indicate what existing standards were used, and how they helped guide the project.
  - 10% An overall picture of the design process (expressed in terms of the design chart), where you highlight the specific connections (connecting lines on the design chart) that you have focused on
  - 40% What you did and what you learned from it. You won't have time to explain all of the results you obtained in detail, but you should be able to articulate in clear terms how you have enhanced the design of your material

10%: Use of Professionally Recognized Standards: Use of standards to define performance metrics and quantify property targets.

20%: Analysis, modeling or experimentation: The details of this part will vary quite a bit from group to group. Some of the general ways to satisfy this requirement include the following:

- ◇ Development of some specific designs and experimental validations of these designs
- ◇ Computational modeling of one or more elements of your design
- ◇ Computational modeling to develop quantitative property metric from the performance metric
- ◇ Use of existing material models for structure/property relationships
- ◇ Modeling of the process in order to achieve the desired structure

10%: Individual contributions

- ◇ This includes overall class presence and participation. Include in your report a list of the team members, with a list of parts of the project that each team member contributed to.

Schedule

The labs and homeworks will be submitted through Canvas, but the detailed schedule for the class is the one posted online:

msecore.northwestern.edu/390/390syllabus.pdf.

The project updates are not expected to take the whole class period, and are meant to be concise PowerPoint presentations outlining what progress has been made so far, and what is planned for the next week. Upload the presentations to Canvas, and specify a lead presenter for each one, rotating through the members of the project team.

	Date	**Topic**	**Assignment** (all but lab upload due before class)
1	Wed. Sep. 25	Intro	
2	Fri. Sep. 27	Software, **Lab 1**	upload last lab page to Canvas
3	Mon. Sep. 30	Standards, Design Chart	

	Date	Topic	Assignment (all but lab upload due before class)
4	Wed. Oct. 2	**Lab 2**	upload last lab page to Canvas **HW 1**
5	Fri. Oct. 4	**Lab Safety, Finalize Initial Experimental Design**	**Overleaf:** Image, Design Chart, Standards, Performance Metrics
6	Mon. Oct. 7		
7	Wed. Oct. 9	**Lab 3**	upload last lab page to Canvas **HW 2**
8	Fri. Oct. 11		**Overleaf:** Property requirements and Materials Selection
9	Mon. Oct. 14	**Project Update 1**	**upload slides to Canvas**
10	Wed. Oct. 16	**Lab 4**	upload last lab page to Canvas **HW 3**
10	Wed. Oct. 16	**Lab 4**	upload last lab page to Canvas **HW 3**
11	Fri. Oct. 18		
12	Mon. Oct. 21	**Project Update 2**	**upload slides to Canvas**
13	Wed. Oct. 23		**HW 4**
14	Fri. Oct. 25		
15	Mon. Oct. 28	**Project Update 3**	**upload slides to Canvas**
16	Wed. Oct. 30		
17	Fri. Nov. 1		
18	Mon. Nov. 4	**Project Update 4 - results from first round of experiments**	**upload slides to Canvas**
19	Wed. Nov. 6		
20	Fri. Nov. 8		
21	Mon. Nov. 11	**Project Update 5**	**upload slides to Canvas**
22	Wed. Nov. 13		

	Date	Topic	Assignment (all but lab upload due before class)
23	Fri. Nov. 15		
24	Mon. Nov. 18	**Project Update 6**	**upload slides to Canvas**
25	Wed. Nov. 20		
26	Fri. Nov. 22		
27	Mon. Nov. 25	**Project Update 7**	**upload slides to Canvas**
28	Wed. Nov. 27		
29	Mon. Dec. 2		
30	Wed. Dec. 4		
31	Fri. Dec. 6	**Final Presentation**	**Upload presentation slides to Canvas**.
	Wed. Dec. 11		**Finalize overleaf file by midnight**.

Assignment Details:

- ◇ The 'labs' are designed to step your through the use of the software in a very straightforward and directed way. These are done in class individually (although you can certainly discuss it with each other) and a screenshot of the completed exercise is uploaded to canvas.
- ◇ The 'homeworks' correspond to each lab, and are due at the beginning of class, one week after the corresponding lab.
- ◇ The final project reports are written collaboratively in Overleaf (one per group) using a template that will be provided to you.

2 Catalog Description

Analysis and control of microstructures. Quantitative process/structure/property/performance relations, with case studies. Computer lab for modeling multicomponent thermodynamics and transformation kinetics. Prerequisites: 315, 316 1,2, or consent of instructor.

3 Course Outcomes

At the conclusion of the course students will be able to:

1. Apply a systems approach to complex problem identification and formulation.

2. Apply property/performance relations to materials selection, and to the specification of property objectives to meet user performance needs in evolving environments.
3. Apply mechanistic models in design integration of process/structure and structure/property relations in dynamic multilevel-structured materials systems
4. Synthesize results of interdisciplinary design research.
5. Apply computational skills in materials selection (CMS Selector), multicomponent thermodynamics (THERMOCALC) and diffusion (DICTRA), and integrate them in the theoretical conceptual design of materials.
6. Perform in cross-functional teams.
7. Communicate effectively in oral, written and graphical form.

4 Introduction

The focus of this class is on the design of a material for a given end use.

We begin with a well-posed performance requirement and design a material to meet that requirement. We'll start by including the Space Elevator as an example, as it illustrates the initial stage in the process, which is to go from a performance requirement (a tether strong enough to connect earth to a satellite in geosynchronous orbit) to the materials requirement (an optimized strength-to-density ratio).

5 Materials Selection: A Case Study

The concept of a space elevator is illustrated in Figure 5.1. The idea is that we run a cable directly from the earth out to a point in space. If the center of mass is at a geosynchronous orbit, the entire assembly orbits the earth at the same angular velocity at which the earth is rotating. To get into space, we no longer need to use a rocket. We can simply 'climb' up the cable at any velocity that we want. The concept is certainly appealing if we can get it to work. But could the concept ever actually work? That is determined by the availability (or lack thereof) of materials with sufficient strength for the cable. We'll need to start with some analysis to figure out what sort of properties are needed.

Consider a mass, m, that is located a distance$r$ from the center of the earth, as illustrated in Figure 5.2. The net force on the object is a centripetal force acting outward (positive in our sign convention) and a gravitational force acting inward (negative in our sign convention):

$$F = m\omega^2 r - G_{gr} M_e m/r^2 \tag{5.1}$$

where G_{gr} is the gravitational constant and M_e is the mass of the earth. The angular velocity of the earth is 2π radians per day, or in more useful units:

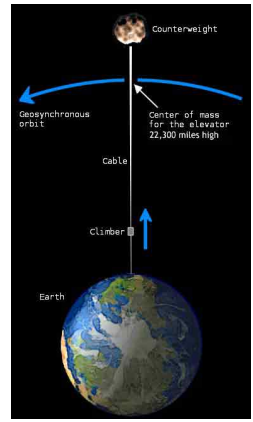


Figure 5.1: Schematic representation of the space elevator.

$$\omega = \frac{2\pi}{(24\,\mathrm{hr})\,(3600\,\mathrm{s/hr})} = 7.3x10^{-5}\,\mathrm{s}^{-1}$$

It is convenient to rewrite the first term in terms of g_0, the gravitational acceleration at $r = r_0$ (at the earth's surface):

$$g_0 = \frac{G_{gr} M_e}{r_0^2} \tag{5.2}$$

The net force on the mass at r can be written as follows:

$$F = m\omega^2 r - m g_0 \left(\frac{r_0}{r}\right)^2 \tag{5.3}$$

The net force is zero for $r = r_s$ (geosynchronous orbit):

$$r_s = \left(\frac{g_0 r_0^2}{\omega^2}\right)^{1/3} = 4.1x10^7\,\mathrm{m}\,(22,000\,\mathrm{miles}) \tag{5.4}$$

This is an easier number to remember than the angular velocity of the earth, so we use this expression for r_s to eliminate ω from Eq. 5.3, obtaining the following:

$$F = m g_0 r_0^2 \left(\frac{r}{r_s^3} - \frac{1}{r^2}\right) \tag{5.5}$$

Now consider a cable that extends from the earths surface ($r = r_0$) to a distance r_ℓ from the earth's surface, as shown in Figure 5.3. We need the cable to be in tension everywhere so that it doesn't buckle. If we design so that the cable is in tension at the earth's surface ($r = r_0$) we're in good shape. The mass increment for a cable of length dr is $\rho A dr$, where A is the cross sectional area of the cable and ρ is the density of the material from which it was made. We obtain the total force, F_0 at the

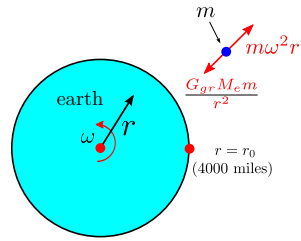


Figure 5.2: Radial forces acting on an orbiting mass.

earth's surface by integrating contributions to the force from the the whole length of the cable:

$$F_0 = \rho A g_0 r_0^2 \int_{r_0}^{r_\ell} \left(\frac{r}{r_s^3} - \frac{1}{r^2} \right) dr \tag{5.6}$$

After integration we get:

$$F_0 = \rho A g_0 r_0^2 \left[\frac{1}{2r_s^3} \left(r_\ell^2 - r_0^2 \right) + \left(\frac{1}{r_\ell} - \frac{1}{r_0} \right) \right] \tag{5.7}$$

F_0 is plotted in Figure 5.4:

Note that the cable is in compression at the earth's surface ($F_0 < 0$) for all values of ℓ less than a critical length r_ℓ, which is equal to 90,000 miles. The maximum tension is at $r = r_s$, and is obtained by integrating contributions to the force from r_s to r_ℓ:

$$F_{max} = \rho A g_0 r_0^2 \left[\left(\frac{1}{r_\ell} - \frac{1}{r_s} \right) + \frac{1}{2r_s^3} \left(r_\ell^2 - r_s^2 \right) \right] \tag{5.8}$$

We have the following numbers:

- $r_0 = 6.4x10^6$ m (4,000 miles)
- $r_s = 4.1x10^7$ m (22,000 miles)

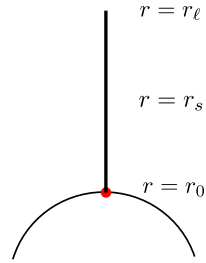


Figure 5.3: A cable extending from the surface of the earth to a distancer_ℓ away from the earth's center.

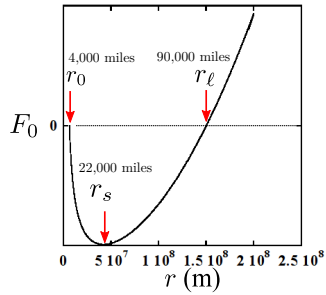


Figure 5.4: F_0 as given by Eq. 5.7.

- $r_\ell = 1.5x10^8$ m (90,000 miles)
- $g_0 = 9.8$ m/s^2

From these numbers we get $\frac{F_{max}}{\rho A} = \frac{\sigma_{max}}{\rho} = 4.8x10^7 \frac{\text{N/m}^2}{\text{Kg/m}^3}$.

Let's compare that to the best materials that are actually available. An Ashby plot of tensile strength (σ_f) and density is shown in Figure 5.5. A line with a slope of 1 on this double logarithmic plot corresponds to a range of materials with a constant value of σ_f/ρ. The line drawn on Figure 5.5 corresponds to σ_f/ρ is≈2.8x10^6 (in Si units), which is the most optimistic value possible for any known material - corresponding to the best attainable properties for diamond. Forgetting about any issues of cost, fracture toughness, etc., we could imagine that we see that we are a factor of 20 below the design requirement. So there's no way this is ever going to work, no matter how good your team of materials scientists is.

All is not lost yet, however, since we really haven't optimized the geometry. The design we considered above has a constant cross-sectional area, which we would really not want to have. What if we optimize the geometry so that material has the largest cross section at $r = r_s$ (where the load is maximized). We'll consider a design where the actual cross section varies in a way that keeps the stress (tensile force divided by cross sectional area) constant. The analysis is a bit more complicated than we want to bother with here, but we get a simple expression for the maximum cross sectional area, A_s (at $r = r_s$), to the cross sectional area at the earth's surface (A_0, at $r = r_0$) :

$$\frac{A_s}{A_0} = \exp\left(\frac{0.77 r_0 \rho g_0}{\sigma}\right) \tag{5.9}$$

If we assume $\sigma/\rho = 2.8x10^6 \frac{\text{N/m}^2}{\text{Kg/m}^3}$, so that the system is operating at the value of σ/f corresponding to the solid line in Figure 5.5 gives $\frac{A_s}{A_0} = 110$. So in this case cable with a diameter of 1 cm at $r = r_0$ needs to have a diameter of ≈ 10 cm at $r = r_s$. We don't have much leeway in decreasing σ/ρ, however. If the best we can do is $\sigma/\rho = 1.0x10^6 \frac{\text{N/m}^2}{\text{Kg/m}^3}$, we get $\frac{A_s}{A_0} = 10^{21}$, which is clearly not workable. So we are stuck with the requirement that the cable have a specific tensile strength equivalent to the best known material on earth without a single critical defect over a length of 90,000 miles. Good luck with that.

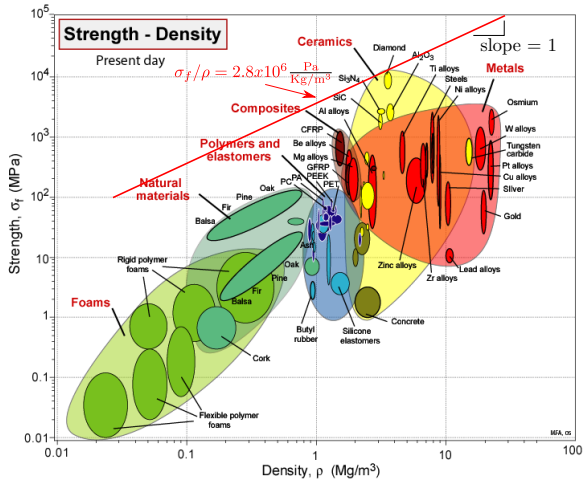


Figure 5.5: Ashby plot of tensile strength and density.

6 Overall Design Approach

The bottom line is that I would NOT want a student group designing a material for a space elevator. However, I could imagine a modified version of the concept where the cable does not extend all the way to the earth's surface, but at least gets us a little bit closer. It's still a pretty esoteric application, but is a useful case for illustrating the sort of things we are looking for in the group design project that is the primary deliverable for the class. Here is some more information about what the final write-up of the design project should include:

6.1 Summary

Here we would describe the concept we are designing the material for, *i.e.* a 'partial' space elevator that can be used to move between different orbital elevations. The results of the analysis presented above would need to be presented here, resulting with the conclusion that we would need to optimize the strength-to-weight ratio.

6.2 Materials Selection

I moved the materials selection section ahead of the system design chart in this case, since it is not immediately obvious what material class will make the most sense for this until we run through the materials selection process. We will probably end up with a carbon fiber reinforced polymer in this case, which will inform our choice of a system chart. Having made the general materials selection, we can use properties of existing materials to figure out how long are cable can actually be. In the context of our example, what values of r_s and r_ℓ will we be assuming in our design?

6.3 System Design Chart

A system chart for a composite material is shown below for the cryogenic liquid storage use case, so our design chart will probably end up looking somewhat like

this the one shown in Figure 6.1. A primary performance characteristic for the partial space elevator would involve structural integrity in the space environment over long periods of time. We'll need to consider things like temperature extremes and effects from radiation damage. In addition to just the tensile strength, we are also going to care about fracture toughness. Processibility will also matter, since we're going to need to make the cable very long. Finally, some consideration of cost needs to be made as well.

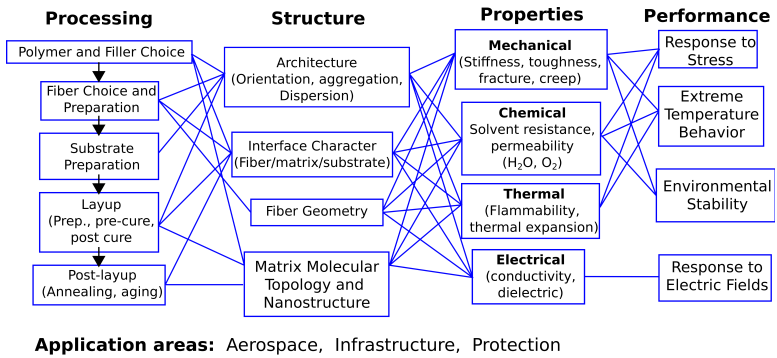


Figure 6.1: System Design Chart for an Aerospace Composite.

A useful tool for developing system design charts has been developed by the Center for Hierarchical Materials Design (CHiMaD) at Northwestern University, and can be accessed at http://chimad-trainings.rcs.northwestern.edu/.

6.4 Design Strategy

This is where the real work takes place. We need to spend some time investigating failure modes of carbon-fiber reinforced polymers, and understand how to design the material appropriate. We need to generally discuss all of the relationships between factors in the design chart, and develop and strategy for optimizing at least one of these factors. We are looking for two elements in your strategy:

1. **A model describing the relationship between structure and the property of interest.** In polymer matrix composites for example, one mode of failure is debonding at the polymer/fiber interface. A tensile stress applied to composite will result in a shear stress at the fiber/matrix interface that can be calculated. Failure can occur either when the stress in the fiber reaches the fracture stress of the fiber, or when the interfacial shear stress exceeds the strength of the interface. This portion of the project will involve investigations of the literature.

2. **Use of a computational tool to address a specific design concern.** This computational tool will likely be either Thermo-Calc or COMSOL. For a composites project, COMSOL will almost certainly be the most useful tool, since it can be used to look at stress distributions within composite structure. Different fiber geometries could be investigated, for example. (Note that many COVID-19 projects will likely utilize composite structures of some

sort (although very different from the rigid, carbon-fiber reinforced polymer composites discussed here.

6.5 Results

Describe the guidance provided by your modeling/computational effort for your overall design. In this case, it may be a description of the most optimal fiber geometry (long, closely packed fibers, shorter fibers with a greater distance between them, *etc.*)

7 Current and Past Projects

7.1 2024 Projects

- ◇ Shape memory alloys for elastocaloric cooling (Darrel Chen, Paloma Lee, Rohan Luthra).
- ◇ Bike wheel spokes (Jake DeRiseis, Joshua Park, Jaemin Yoo).
- ◇ Turbine blade (Jiaqi Shen, Run Yuan, Zixu Xiao).
- ◇ Frames for electric vehicles (Xinzhi Hu, Haojun Xie, Zipeng Xu)
- ◇ Deep Sea Mining (Leif Gregory, Marcos Morales-Martinez, Thomas Zeng)
- ◇ Sustainable Concrete (Camille Layden, Janice Xie)

7.2 2023 Projects

- ◇ Lunar Landing Pads
- ◇ Damage Sensing Composites for Airplane Nosecones
- ◇ Optimization and Design of Metal Heat Shields for CubeSat Rentry
- ◇ Electric Vehicle Battery Casing
- ◇ Underwater Pipelines
- ◇ Experimental Fabrication and Performance Modelling of Flexible Wrist-Worn Biosensors
- ◇ Design of Functionally Graded Materials via Metal Additive Manufacturing

7.3 2022 Projects

These are the projects from 2022. They are the best examples of what is expected in 2023, since the class was fully in-person, and substantial experimental contributions to the projects were possible.

- ◇ Concrete Canoe
- ◇ Mission to Venus
- ◇ Battery Separators

- ◇ Biosensors
- ◇ Cylinder Heads
- ◇ Solid Oxide Fuel Cells

The projects from 2020 and 2021 are given below. The class was taught remotely both years. In 2020 no experimental component was possible, but some of the 2021 projects did include an experimental component.

7.4 2021 Projects

- ◇ 3D Printing
- ◇ Composites for Vehicles
- ◇ Hypersonic Rockets
- ◇ Impact Mitigation
- ◇ Sea Sponges
- ◇ Thermoelectrics

7.5 2020 Projects

- ◇ Additive Manufacturing
- ◇ Antiviral Surfaces
- ◇ Cobalt Alloys
- ◇ Composites
- ◇ COVID PPE
- ◇ N95 Masks
- ◇ Nasal Swabs

8 390 Labs

8.1 Lab 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,

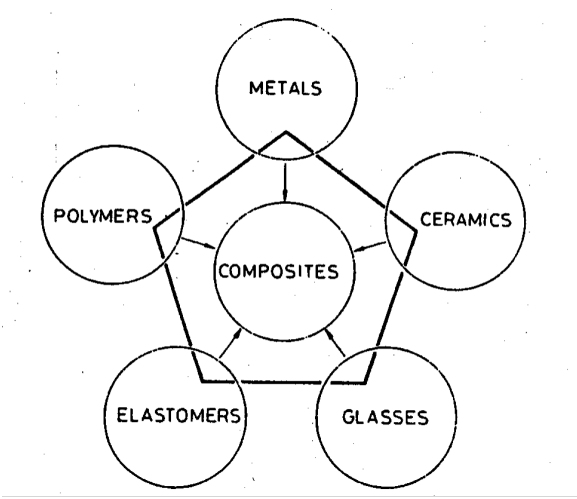
   M = material properties,

   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!).

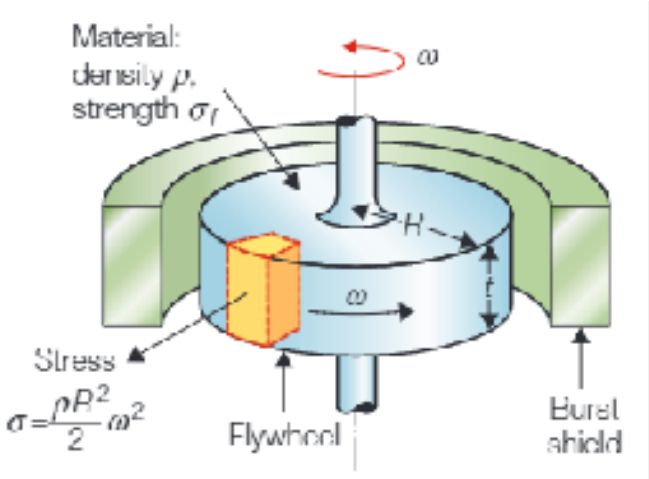
9. How does it work?
   - ◇ Application of set theory and relational algebra

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:

$$U = \frac{J\omega^2}{2} \tag{8.1}$$

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

$$J = \frac{\pi}{4}\rho R^4 t^2 \tag{8.2}$$

The mass of the disk, m, is:

$$m = \pi \rho R^2 t \tag{8.3}$$

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

$$\frac{U}{m} = \frac{R^2 \omega^2}{4} \tag{8.4}$$

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

$$\sigma_{max} = \frac{3+U}{8} \rho R^2 \omega^2 \tag{8.5}$$

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:

$$\frac{U}{m} = \frac{2}{S\,(3+U)} \frac{\sigma_f}{\rho} \tag{8.6}$$

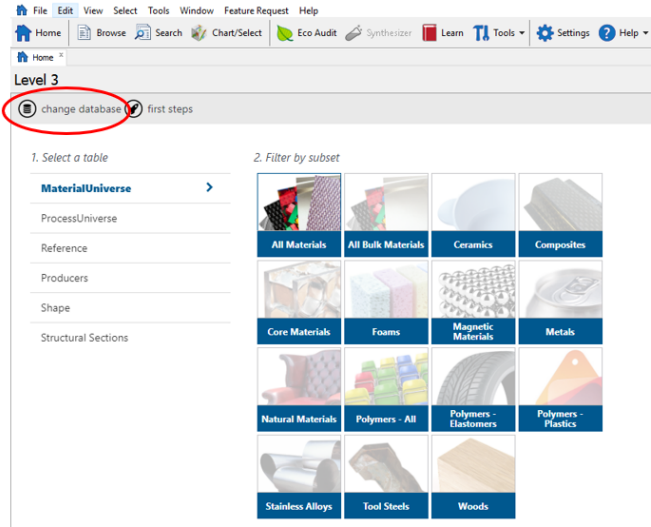
Assuming Poisson's ratio to be constant, the performance index (M) is given as:

$$M = \frac{\sigma_f}{\rho} \tag{8.7}$$

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.

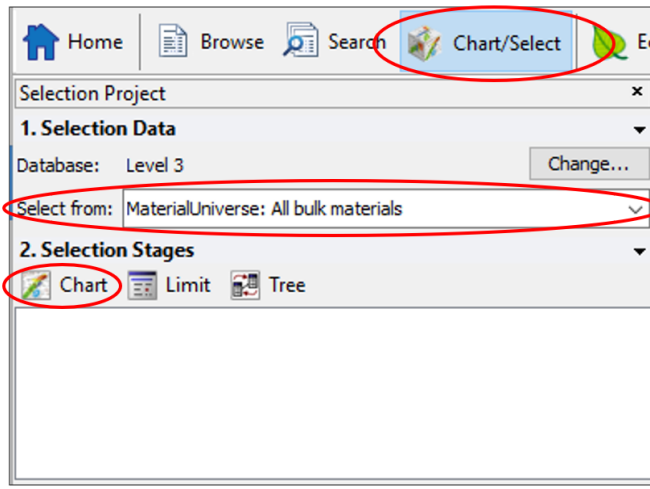
We can now use CES to determine which materials meet these requirements.

- ◇ 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:**



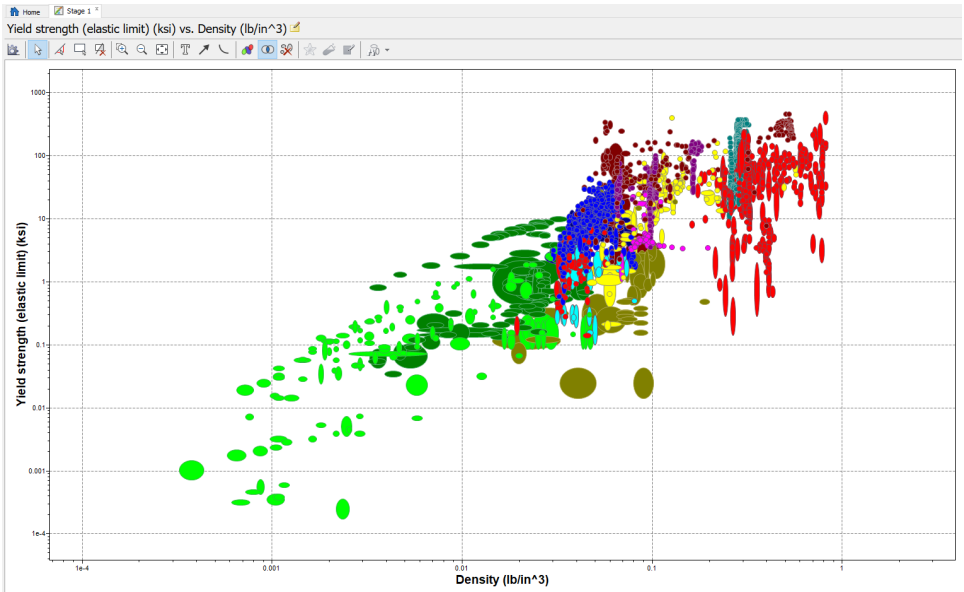
A window entitled "Chart Stage" will appear.

- ◇ 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").

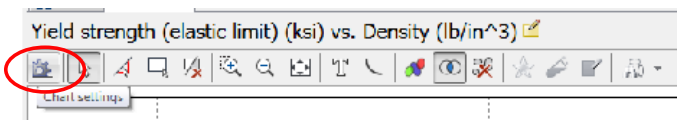
– Note that the default scale for the scale is "logarithmic", which is generally what you want.

◇ 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:



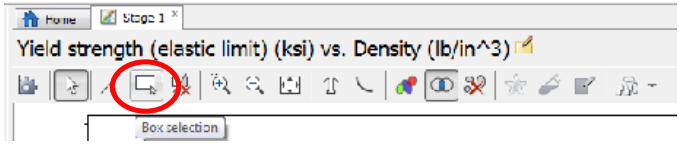
Because the properties of most materials cover a very wide range of values, it is almost always desirable to plot the charts with log scales. This is the default for CES. You can change the scales to linear and back again by clicking on the Stage Properties button (indicated below) in the toolbar and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

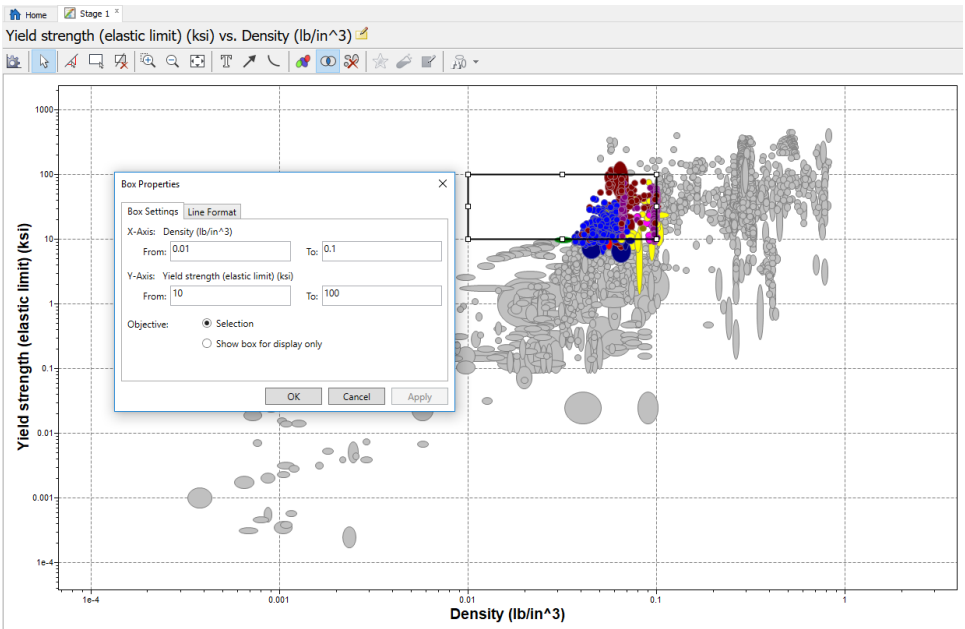
Selecting a subset of materials in a box The simplest way to select a subset of materials from the chart is to draw a 'box' around the ones you want. The procedure for doing this is as follows:

◇ 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:



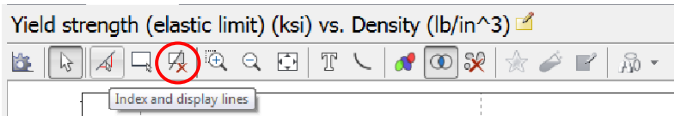
The materials in the box and all the materials that cross the boundary of the box are now plotted in color. This indicates that they have been included in the current subset of materials - they have 'passed' the selection stage. Materials failing the selection stage are plotted in gray. To hide the failed 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. 8.7):

$$M = \frac{\sigma_f}{\rho} \tag{8.8}$$

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

$$\log M = \log \sigma_f - \log \rho \tag{8.9}$$

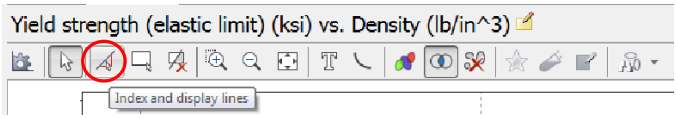
Re-arranging:

$$\log \sigma_f = \log M + \log \rho \tag{8.10}$$

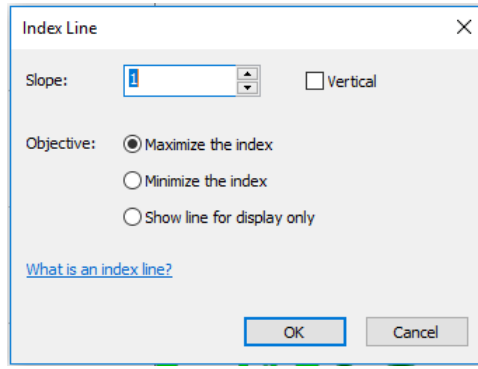
This equation can be plotted as a line of slope 1.0 on a log-log plot of σ_f vs. ρ. All materials lying on this line have the same value of M, and therefore, are equally good for a flywheel. Materials above the line have a higher value of M and perform better.

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

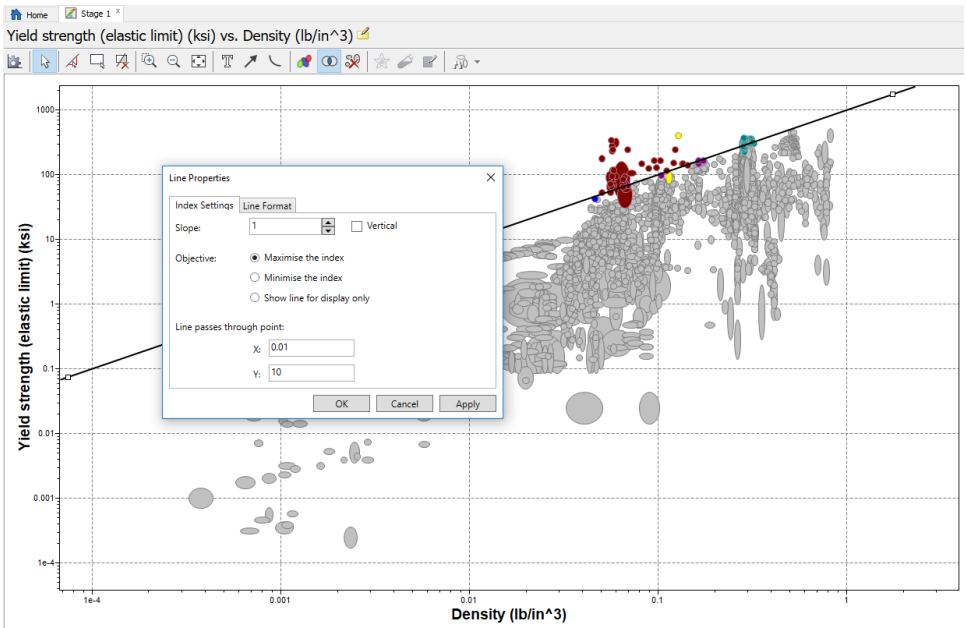
- ◇ Click once on the Index and Display lines button on the toolbar:



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

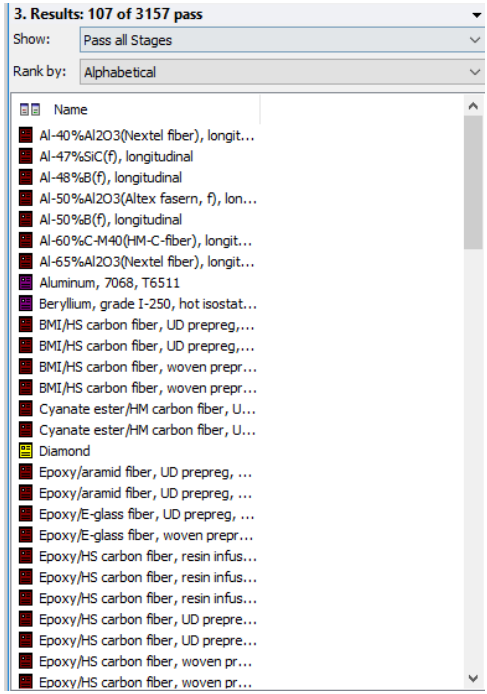


- ◇ Input Slope value 1.
- ◇ Select "Maximize the index".
- ◇ Click on OK.
- ◇ Now pick the point on the chart where the density is 0.01 lb/in3 and the elastic limit is 10 ksi:
  - Click once on the chart to display the line
  - Right click the line and select "Properties"
  - Input the point value (X: 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:



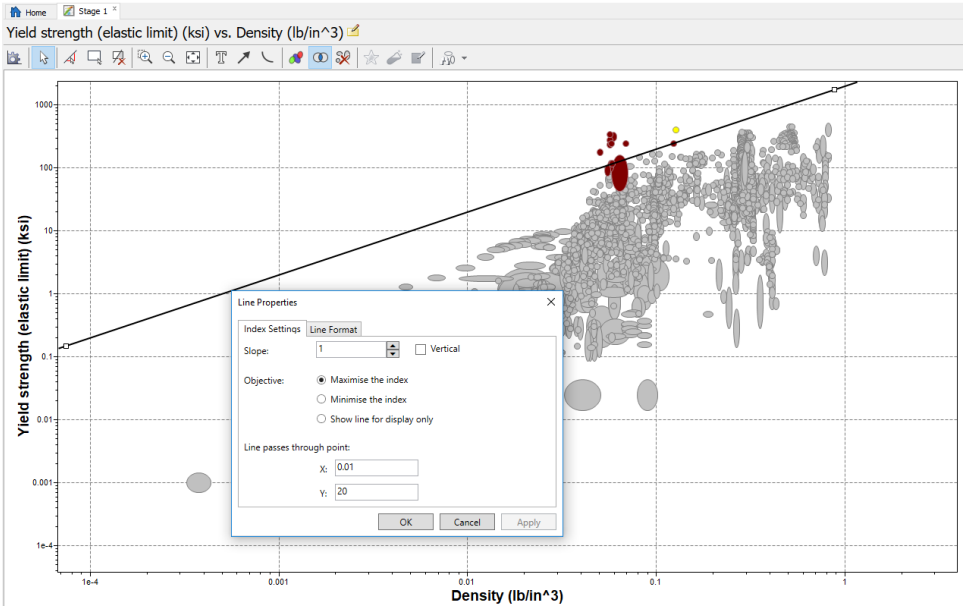
The contents of the Results window show that 107 out of 3157 materials in the MaterialsUniverse database passed the stage 1 selection (results may be slightly different, depending upon the exact position of your selection line and your version of the database). Double-clicking on any of the materials 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/

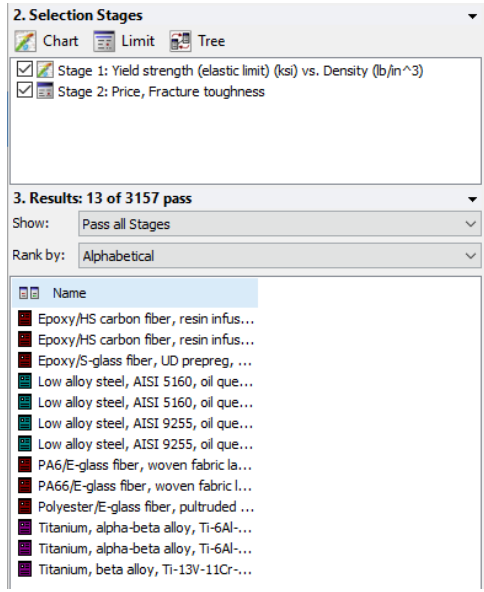
The bubble will now flash on and off, and a temporary label will appear on the screen. When you double click on a material, the property information pops up in the Properties window. The Properties window will now display the properties of the material that you selected on the chart.

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:

$$M = \frac{\left(10^9\,\mathrm{Pa}\right)^{1/2}}{1000\,\mathrm{kg/m^3}} = \frac{(1000\,\mathrm{Pa})^{1/2}}{\mathrm{kg/m^3}} \tag{8.11}$$

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.

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

8.2.1 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.

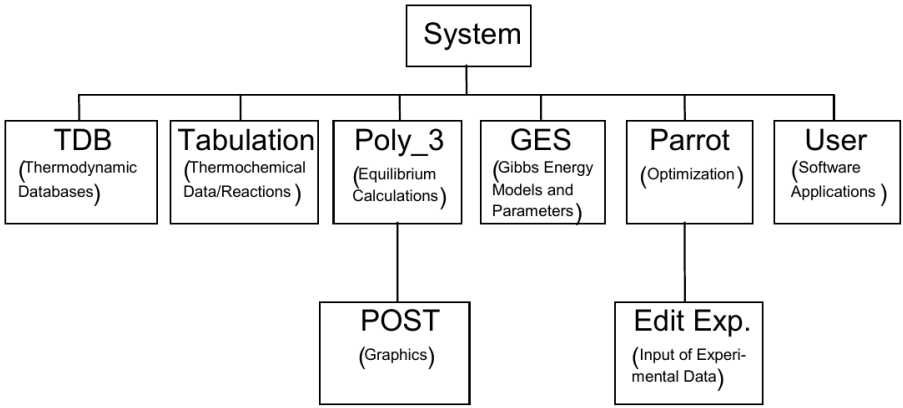
3. Applications
   - ◇ Materials processing
   - ◇ Materials design

8.2.2 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

8.2.3 Modular Character of Thermo-Calc

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



8.2.4 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.

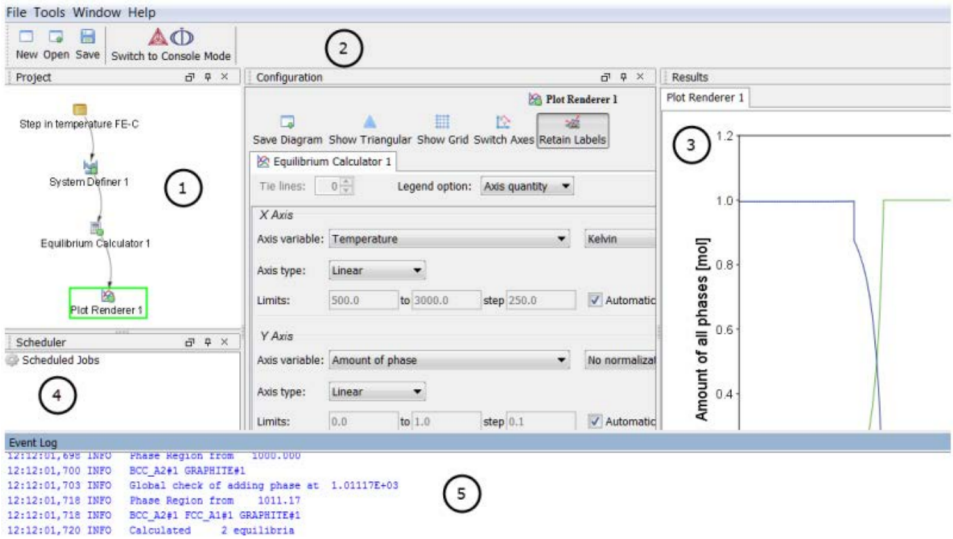
Species: The collection of all constituents for the phases in a given system and can be elements, molecular aggregates, charged or neutral.

8.2.5 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.



8.2.6 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

8.2.7 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.

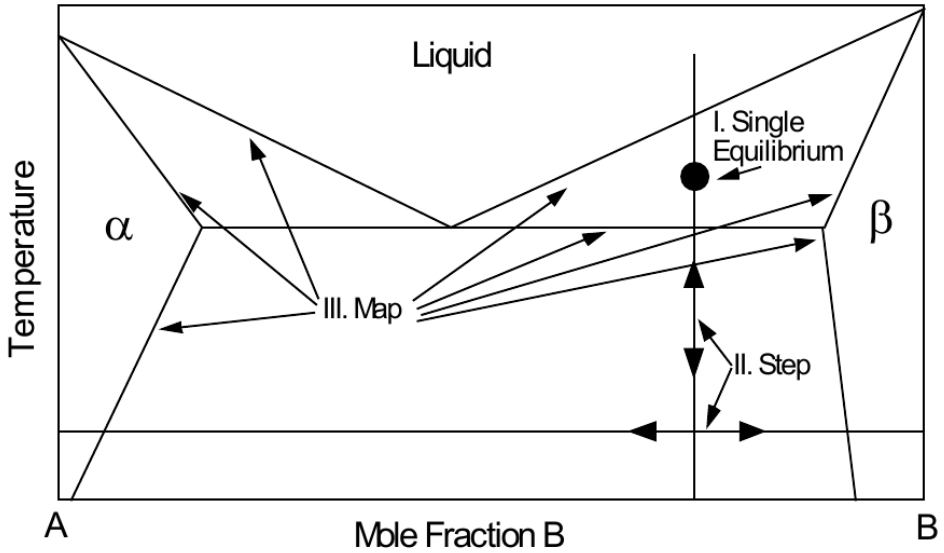
- ◇ Typically the size of the overall system must be constrained by setting the number of moles in the system equal to 1.
- ◇ Functions of state variables can also be used as conditions, but must be posed such that the function equals 0.

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.

8.2.8 Types of Calculations in POLY3 Module

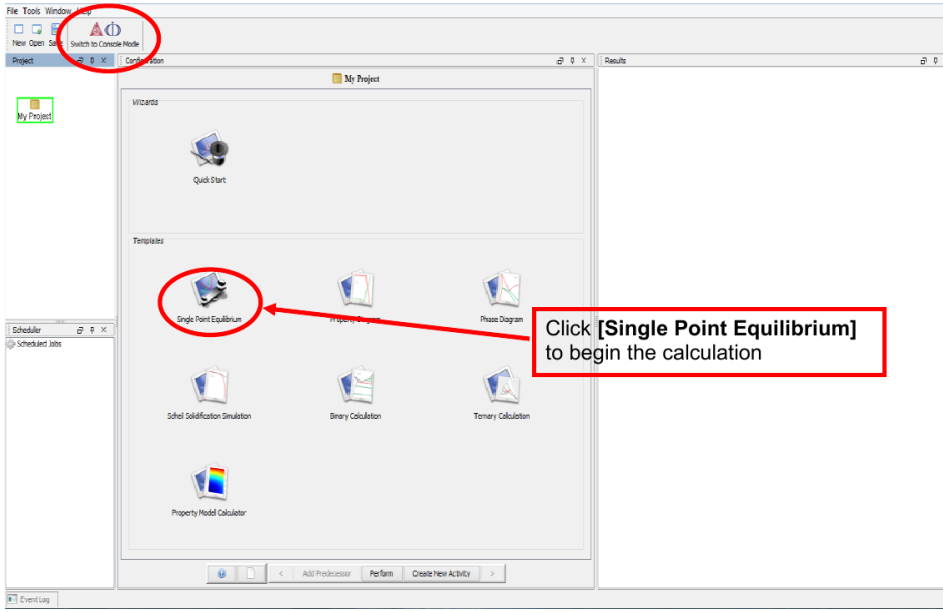


- ◇ I. Single Equilibrium (Single Point Calculation): Nothing is varied
- ◇ II. Step Calculation (Property Diagram): One state variable is varied
- ◇ III. Map Calculation (Phase Diagram): Two state variables are varied

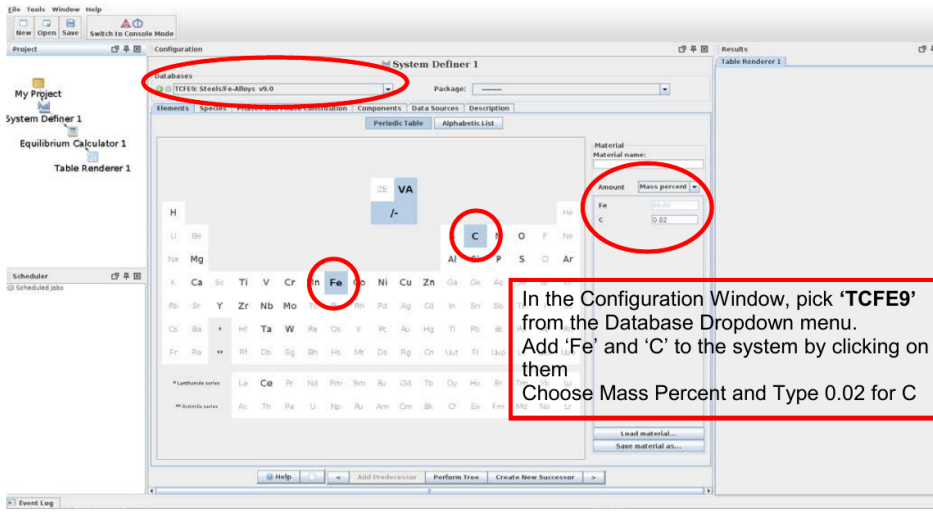
8.2.9 EXAMPLE 1: Single Point Calculation of Fe-0.02C (wt%) at $T = 800\,^{\circ}\mathbf{C}$

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

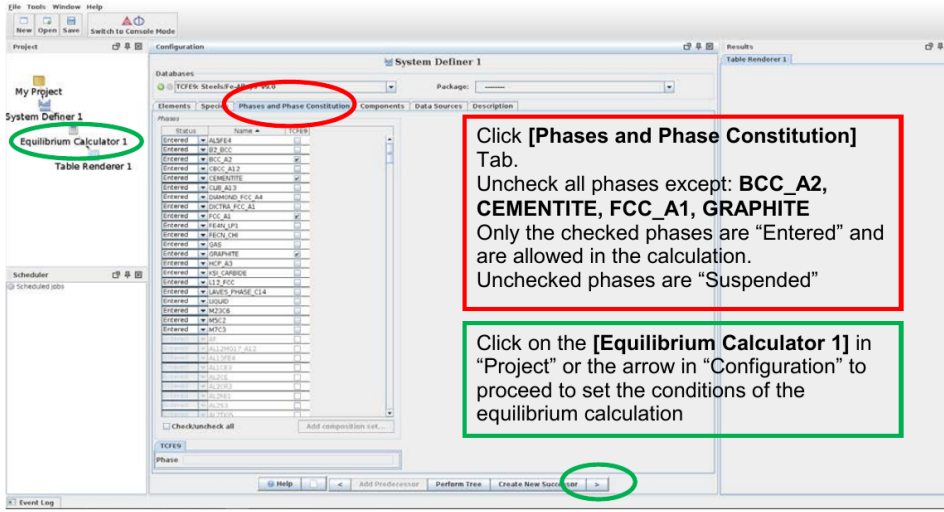
1. Open TC2021b and enter GUI mode. Select 'Single Point Equilibrium'



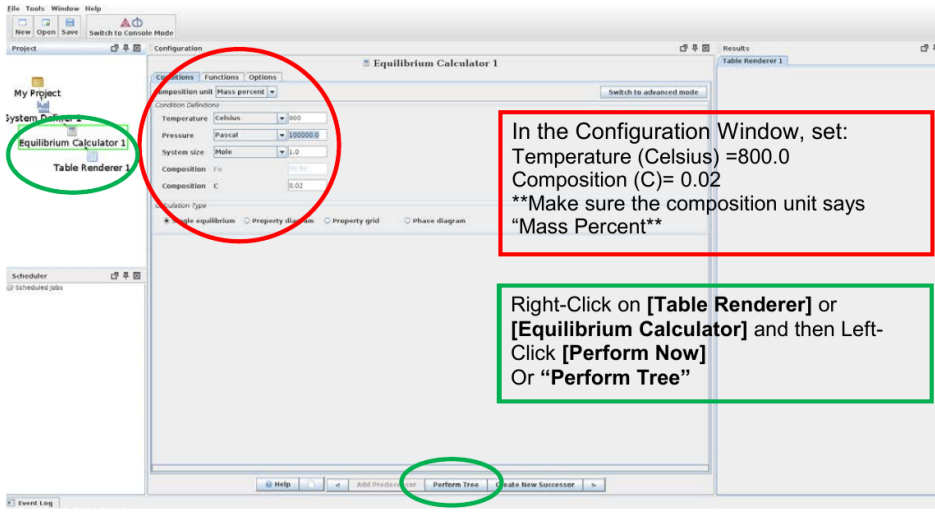
2. System Definer 1 - Pick Database and Elements in System



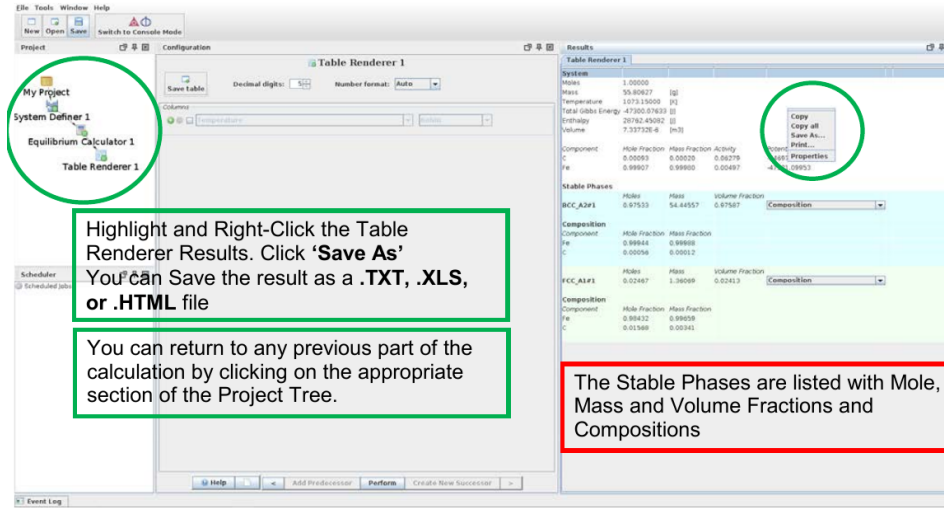
3. System Definer 1 - Identify Phases and Phase Constitution in System



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



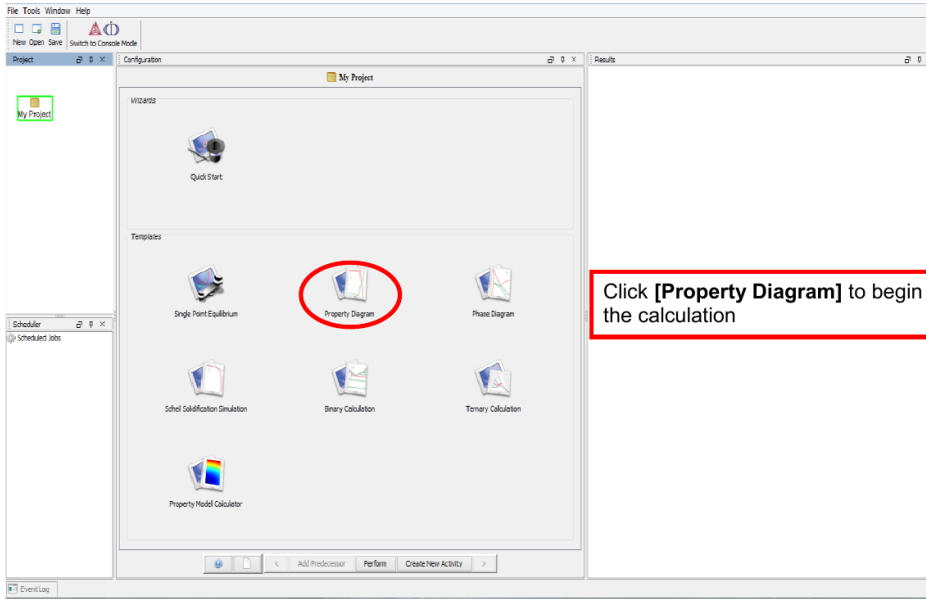
8.2.10 EXAMPLE 2: Step Calculation for a Dilute Al-Mn-Ge-Si Alloy

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.

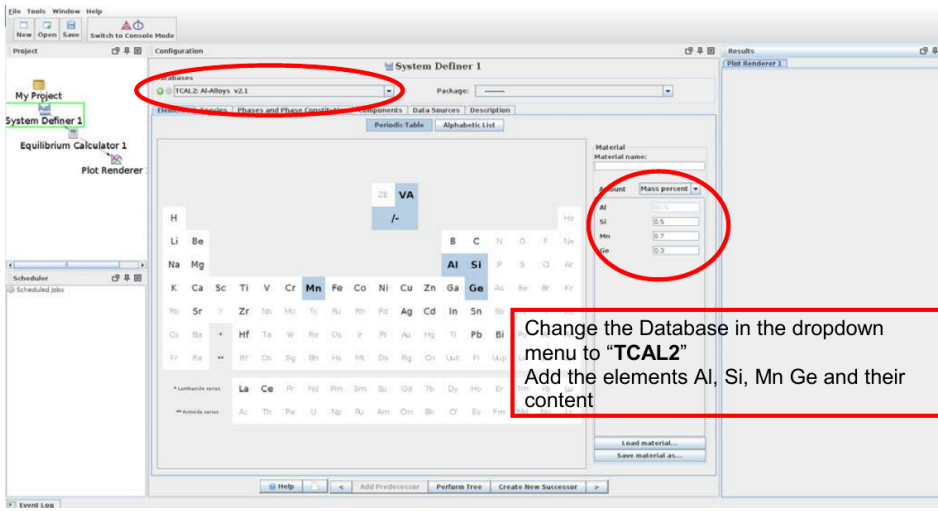
In this example, we will use an Al-0.7Mn-0.5Si-0.3Ge (wt%) alloy. We want to find out what is its solution treatment temperature (i.e., the temperature at which all solutes are dissolved in Al). We also want to know what the equilibrium phase(s) are at various aging temperatures.

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

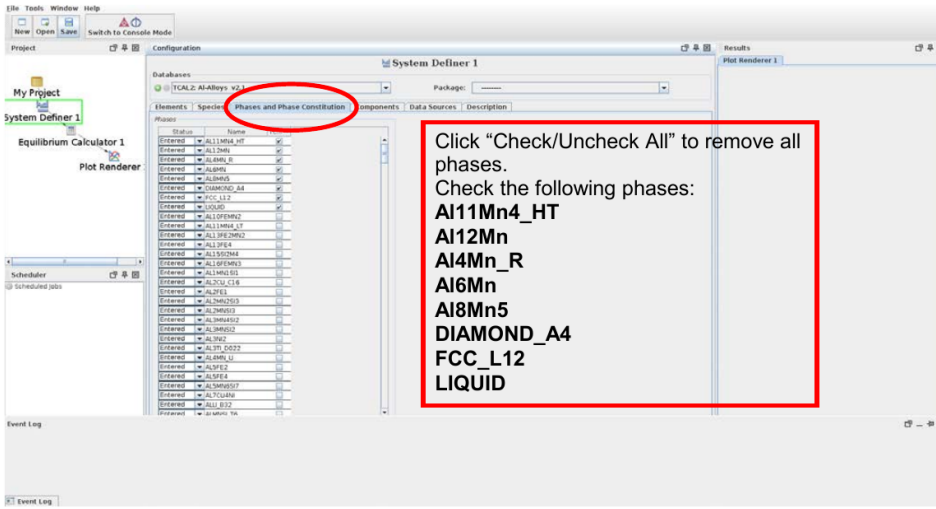
Step 1: Open TC2017b and enter GUI mode. Select 'Property Diagram'



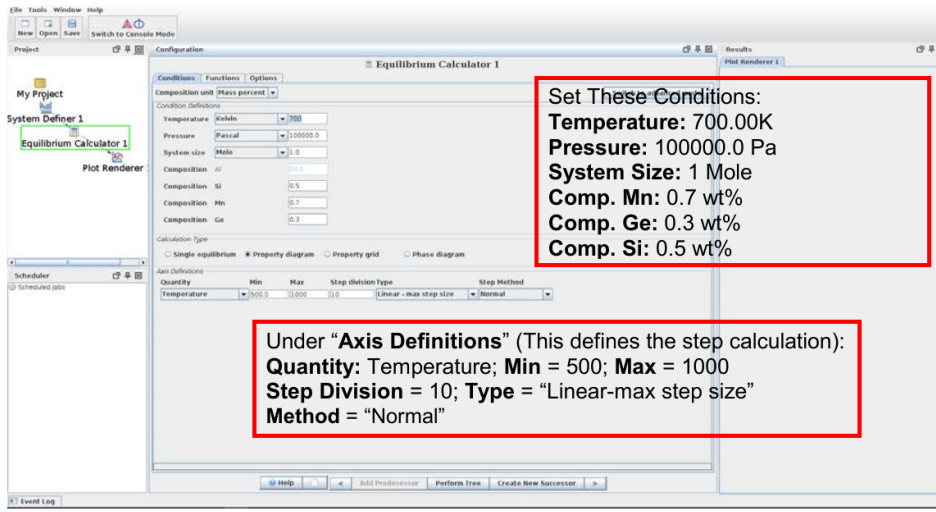
2. Change the database, add the correct elements, go to the Phases tab.



3. Choose Phases.

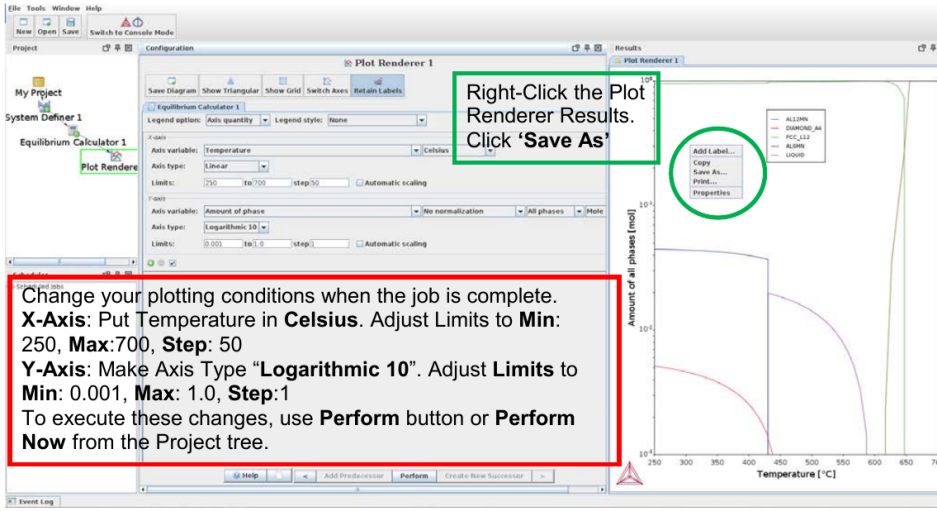


4. Set Conditions (Temperature and Composition). Then Perform calculation.

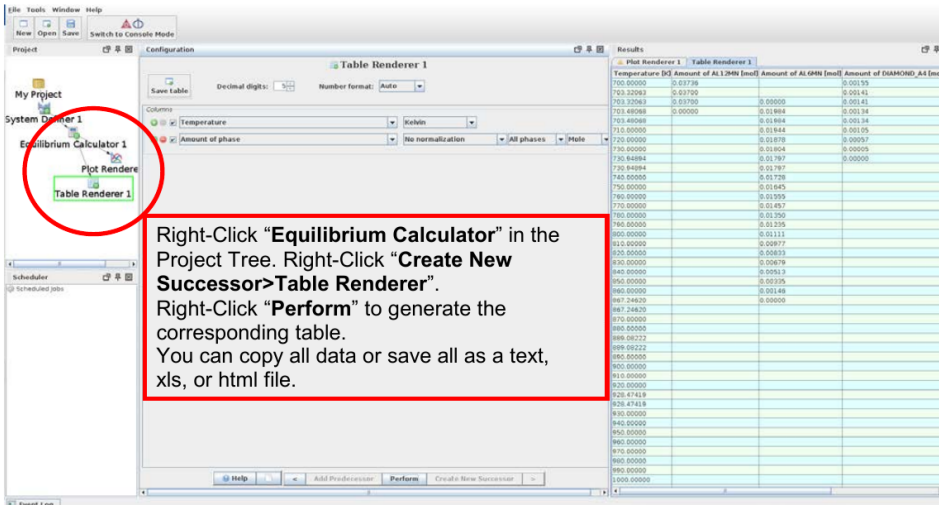


5. Plot Renderer Results and Save the Diagram or Data Table.

   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".

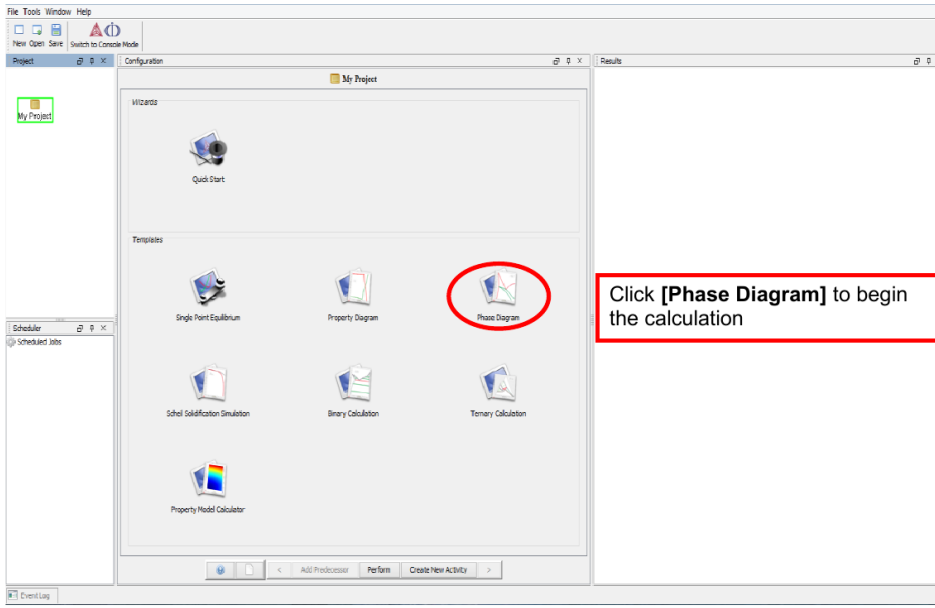


8.2.11 EXAMPLE 3: Map Calculation for a Fe-C Metastable Phase Diagram

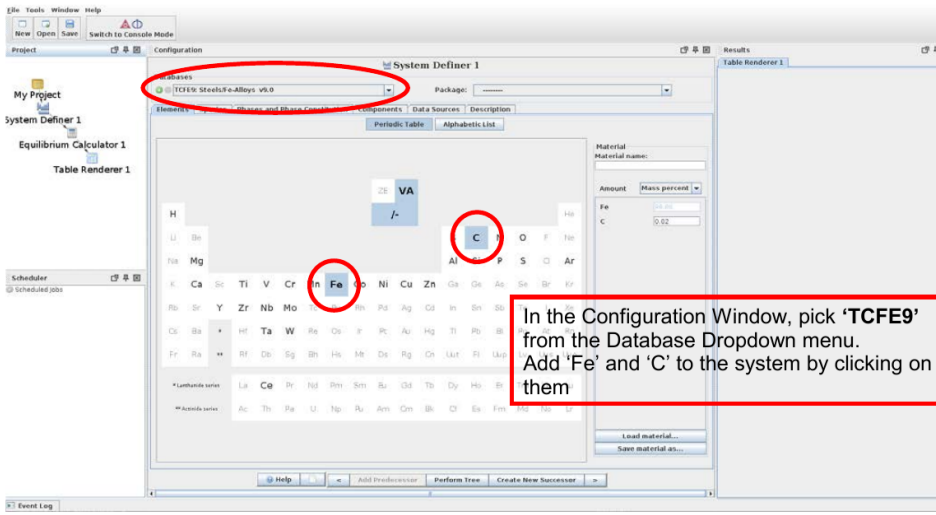
Mapping Calculations allow variation of two variables. These enable the calculation of phase diagrams (varying Temperature and Composition). For this example, we'll calculate a metastable equilibrium diagram of Fe-C.

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

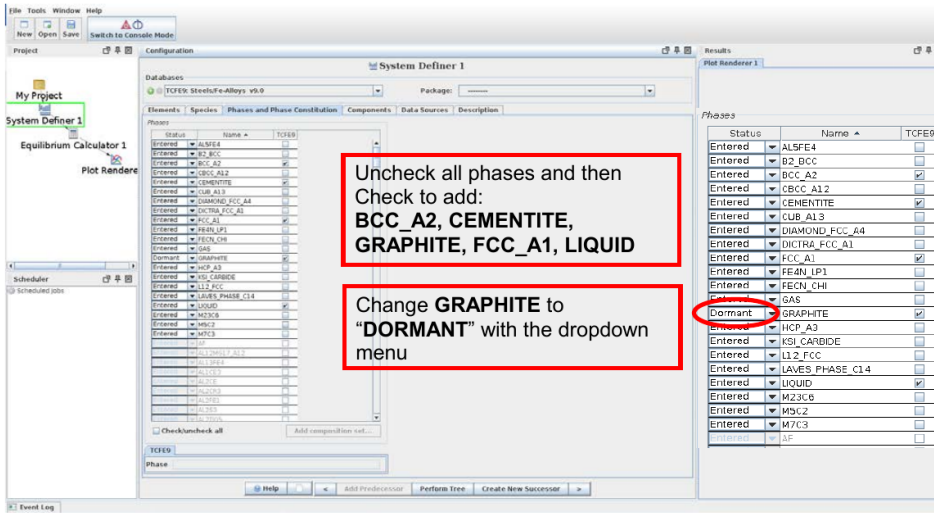
   Binary Calculator or Ternary Calculator are quick templates for Binary and Ternary Diagrams but feature less customizability.



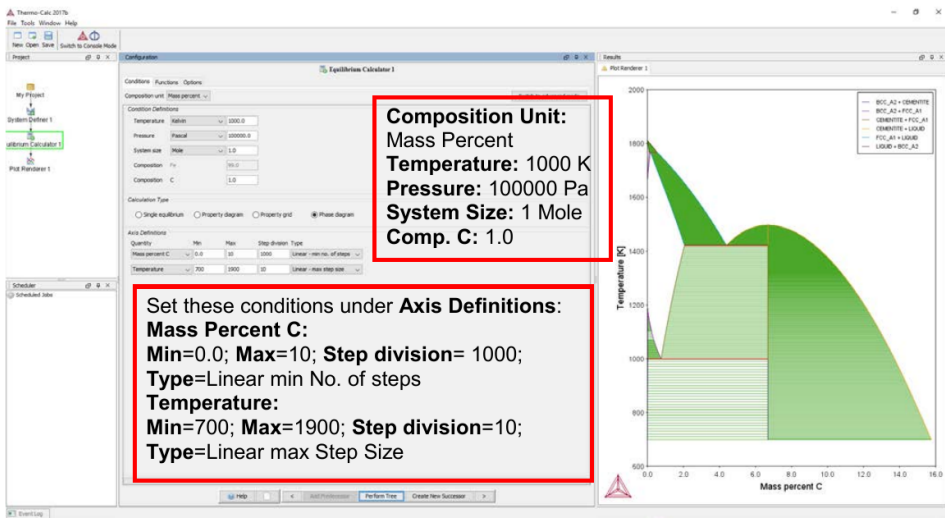
2. Choose the Correct Database and add Elements



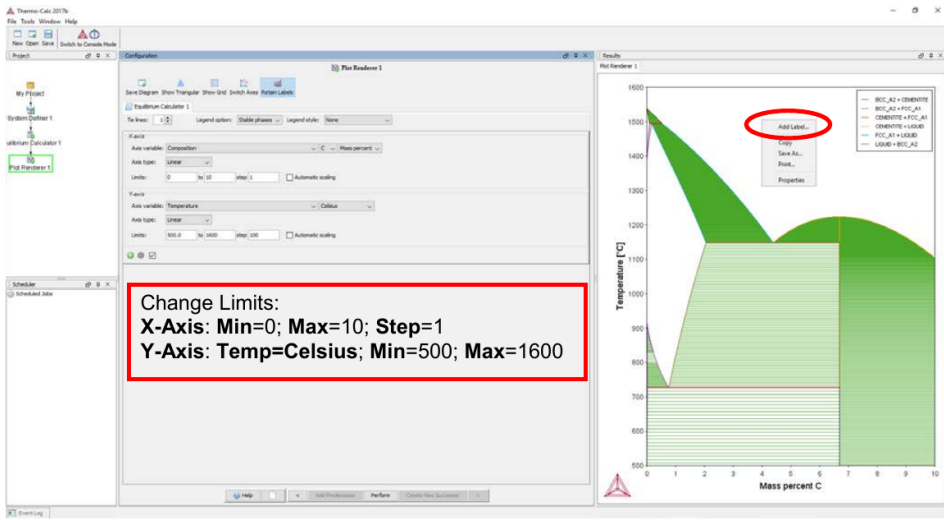
3. Add Phases and Make Graphite Dormant



4. Set Mapping Conditions, Then Perform calculation

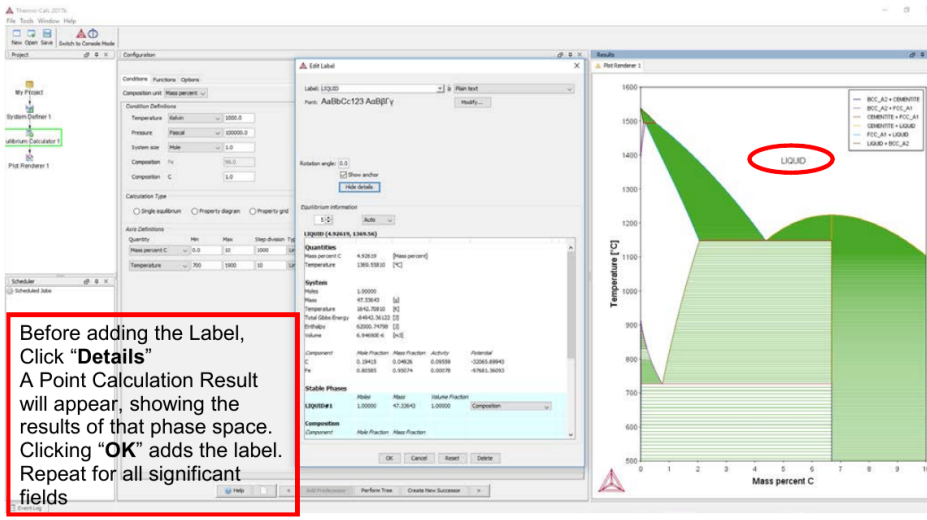


5. Change Axis Limits. Insert Labels.



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.

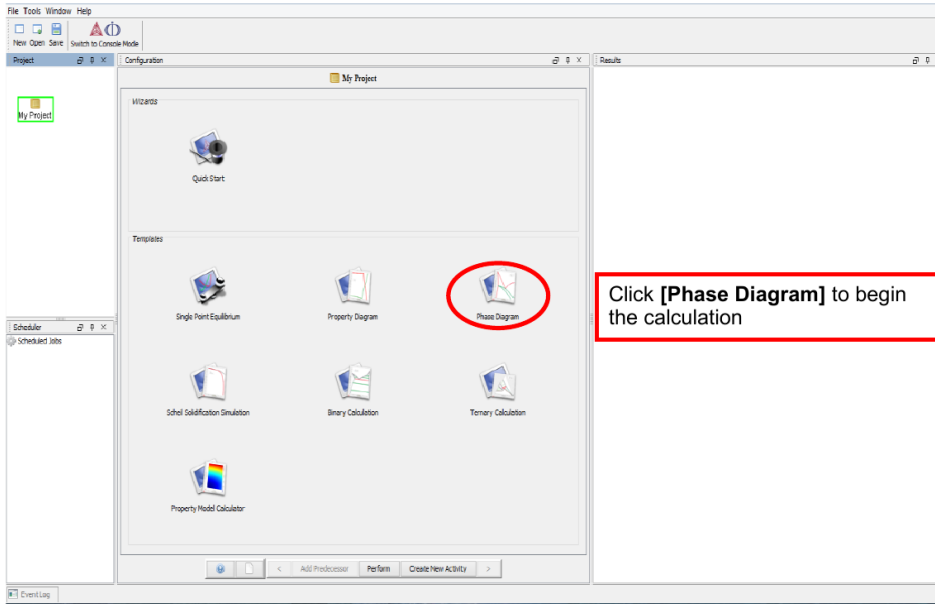


8.2.12 EXAMPLE 4: Calculate an Isothermal Section of Fe-Ni-Cr system at 600 °C

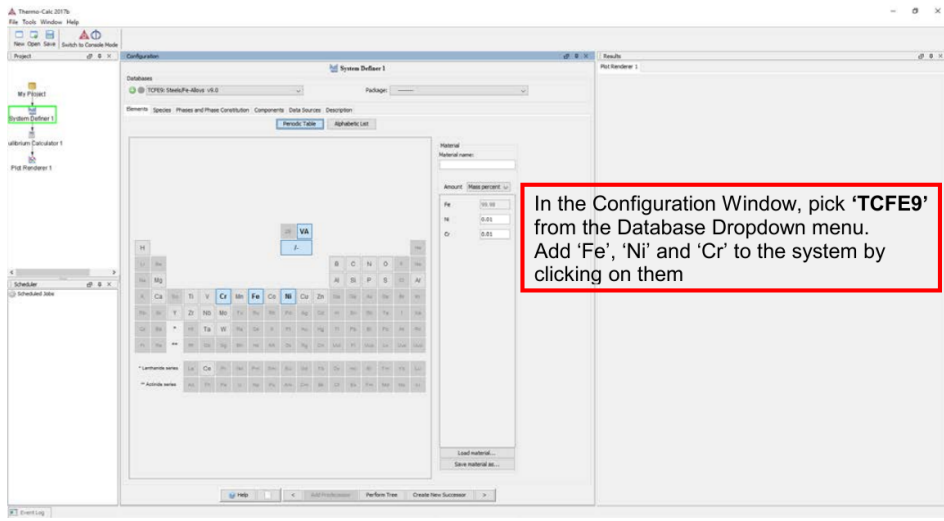
An isothermal section of the ternary system provides us the composition-phase roadmap at a particular temperature. This information is very useful in selecting alloy compositions, knowing the equilibrium phases present, their amounts and compositions for a given alloy composition etc. The phase equilibria 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.

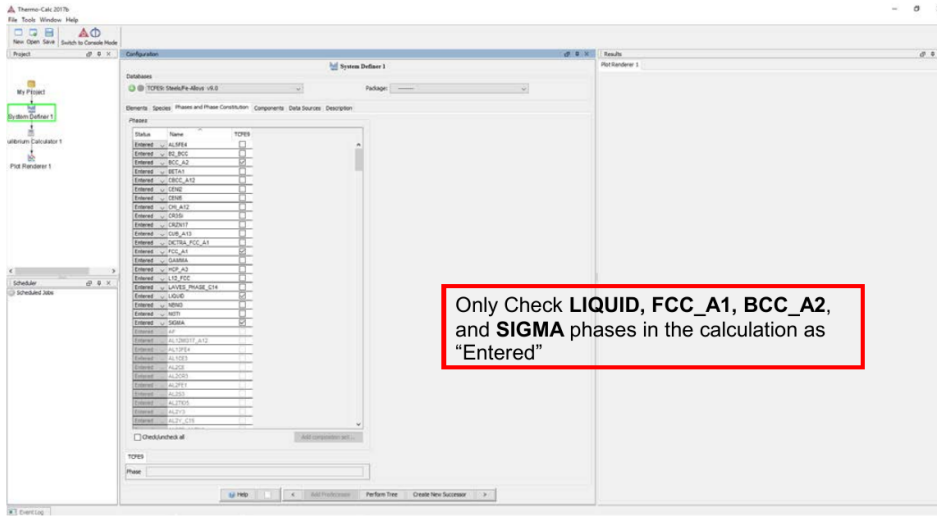
1. Open TC2021b and enter GUI mode. Select 'Phase Diagram'



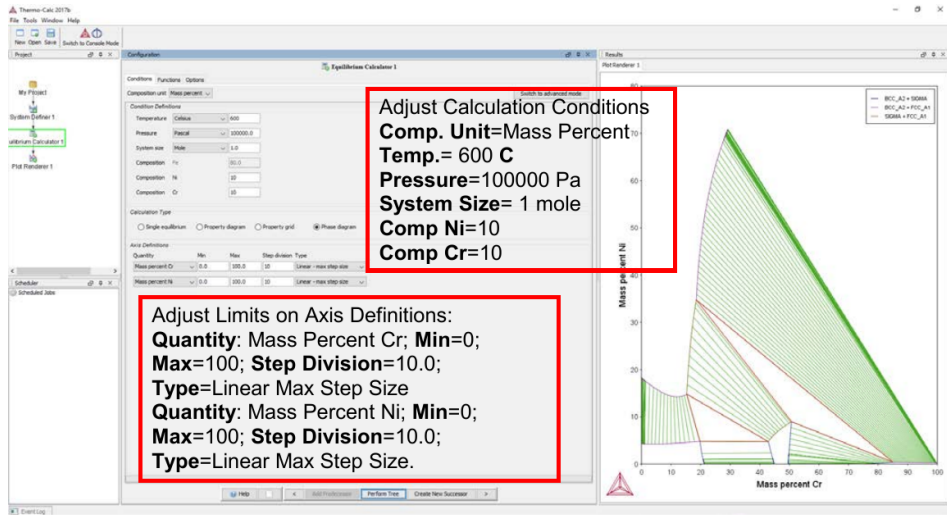
2. Choose the Correct Database and add Elements



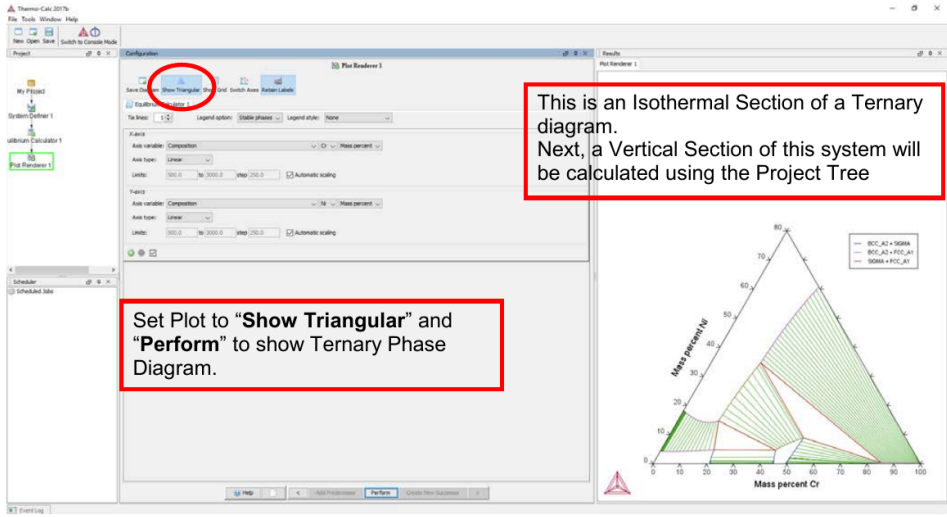
3. Add Phases



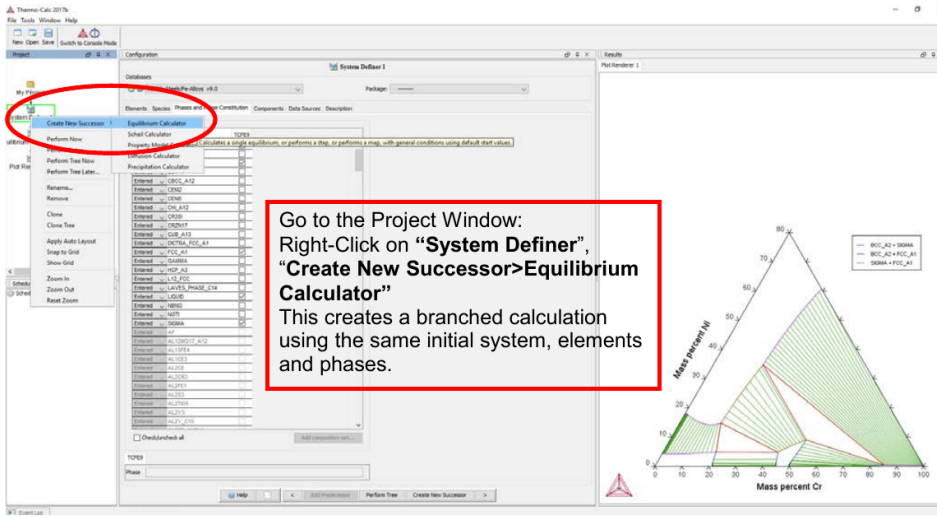
4. Set conditions, then perform calculation.



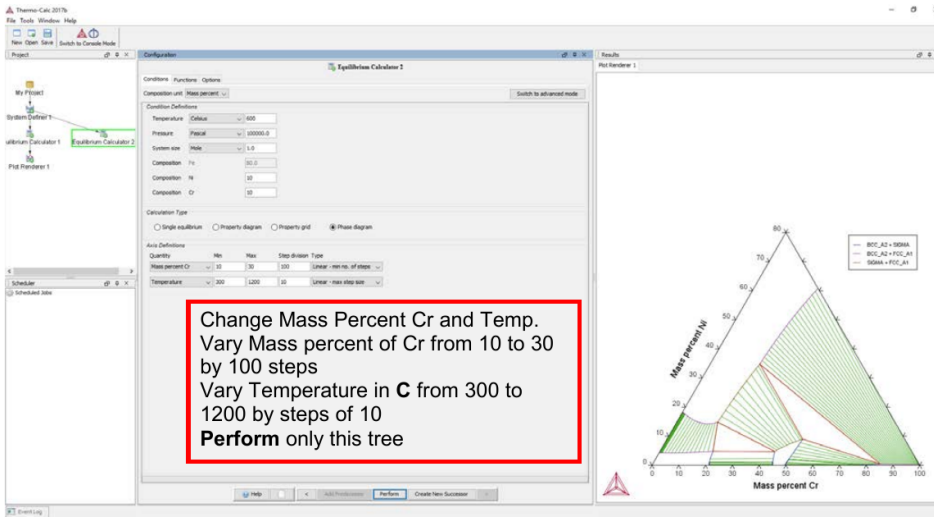
5. Finish the plot as a triangular diagram.



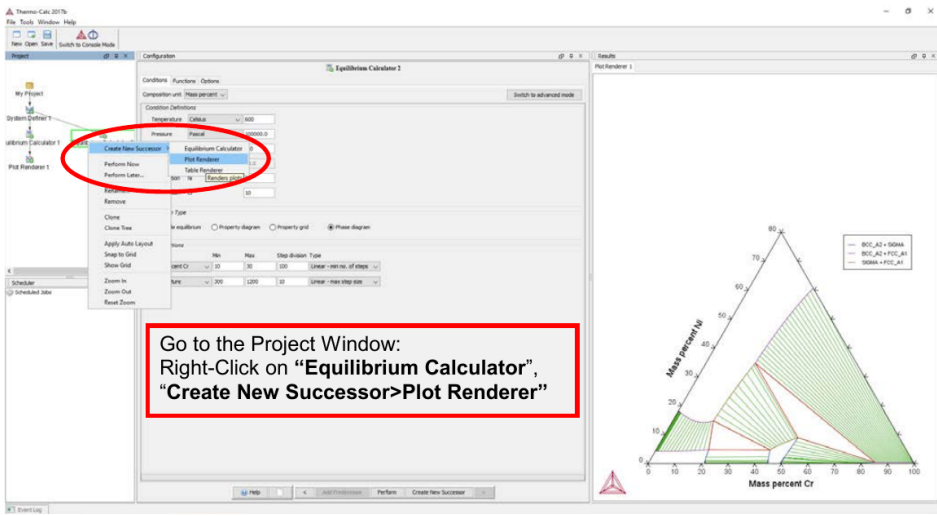
6. Create a new Branch of the Project.



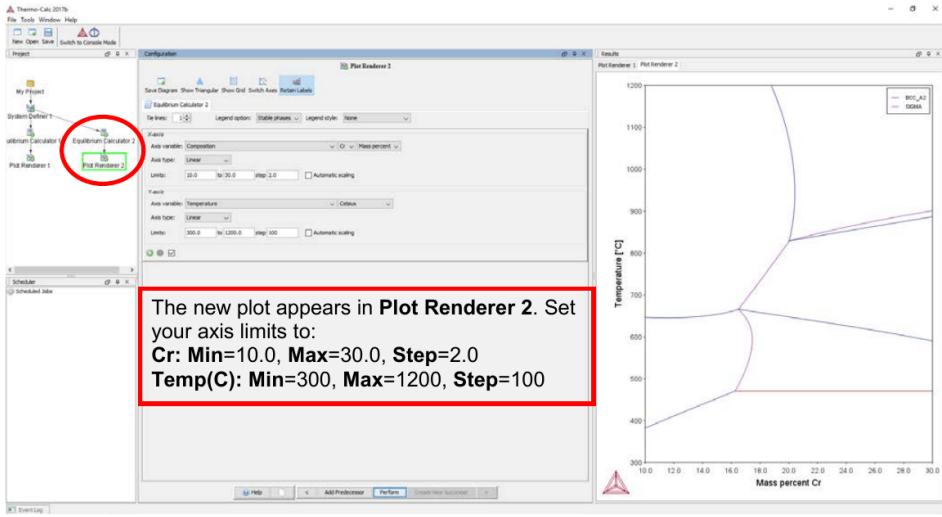
7. Set Conditions and Perform Equilibrium Calculations

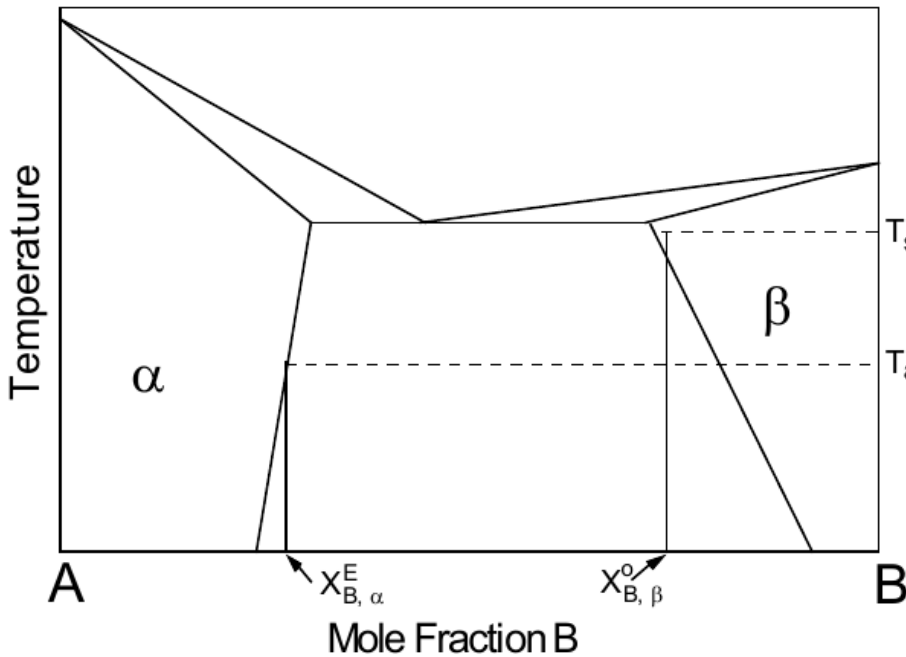


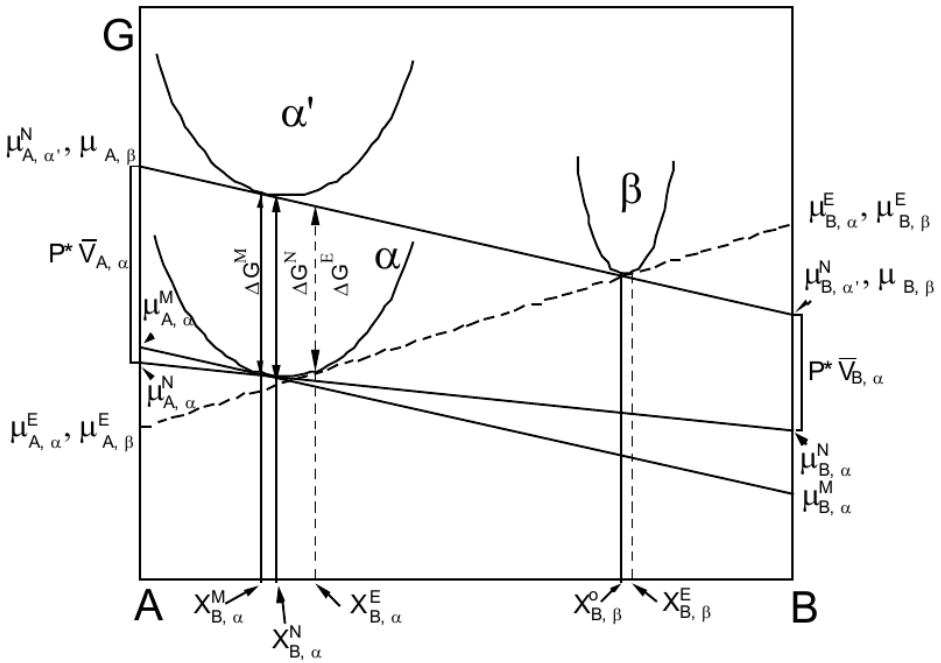
8. Create a new Plot Renderer

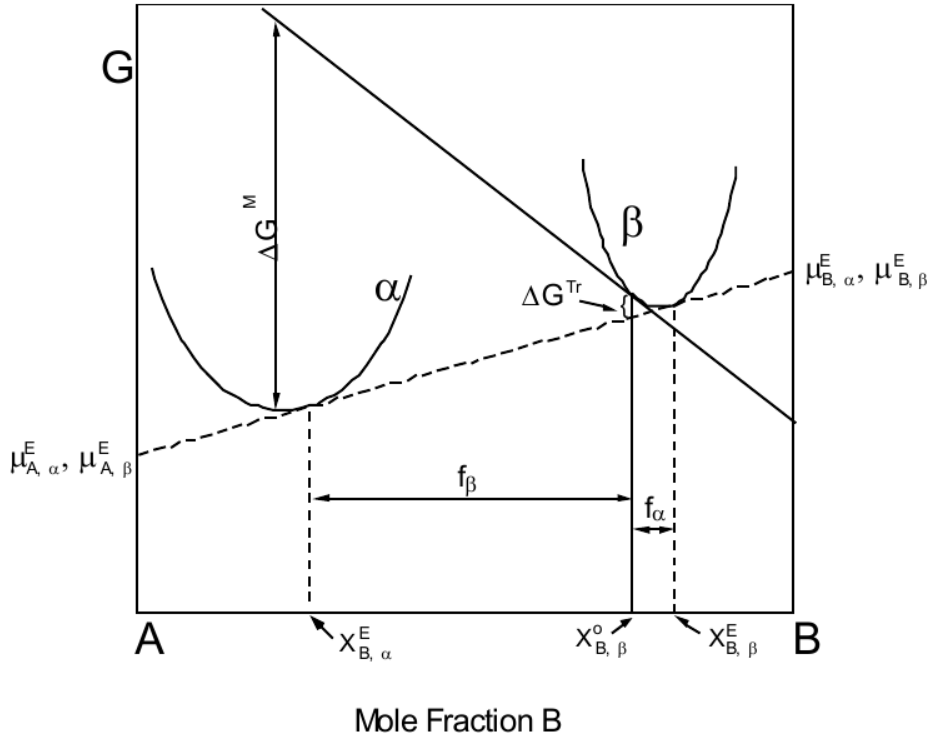


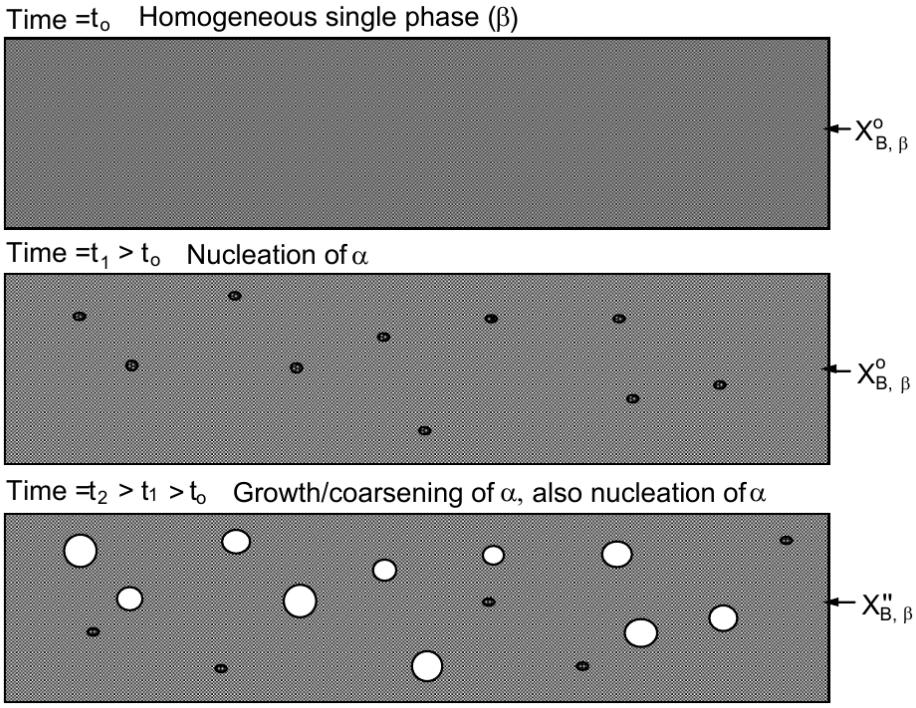
9. Create a new Plot Renderer, Set Plot Axis and Perform


The new plot appears in **Plot Renderer 2**. Set your axis limits to:
Cr: Min=10.0, **Max**=30.0, **Step**=2.0
Temp(C): Min=300, **Max**=1200, **Step**=100
Temperature [°C]
Mass percent Cr


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


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

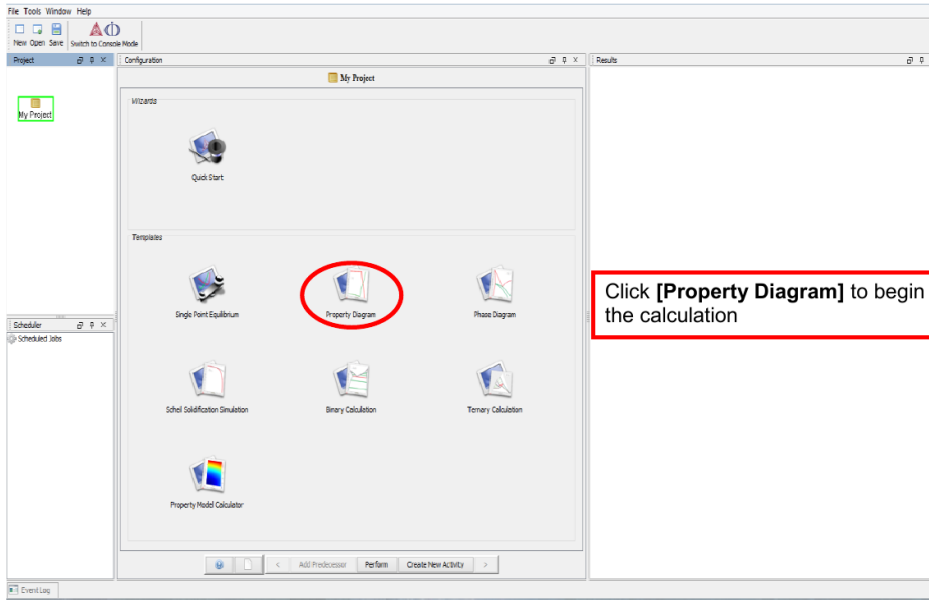

G
ΔG^M
α
β
ΔG^{Tr}
$\mu^E_{B,\alpha}, \mu^E_{B,\beta}$
$\mu^E_{A,\alpha}, \mu^E_{A,\beta}$
f_β
f_α
A
$X^E_{B,\alpha}$
$X^o_{B,\beta}$
$X^E_{B,\beta}$
B
Mole Fraction B



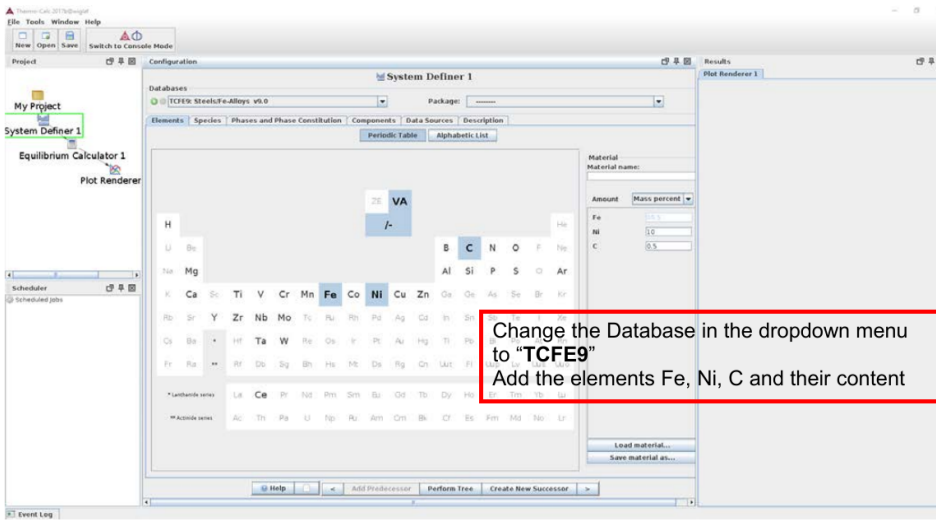
8.2.13 EXAMPLE 5: Composition-Invariant Transformation

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 ($DeltaG_m$ 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.

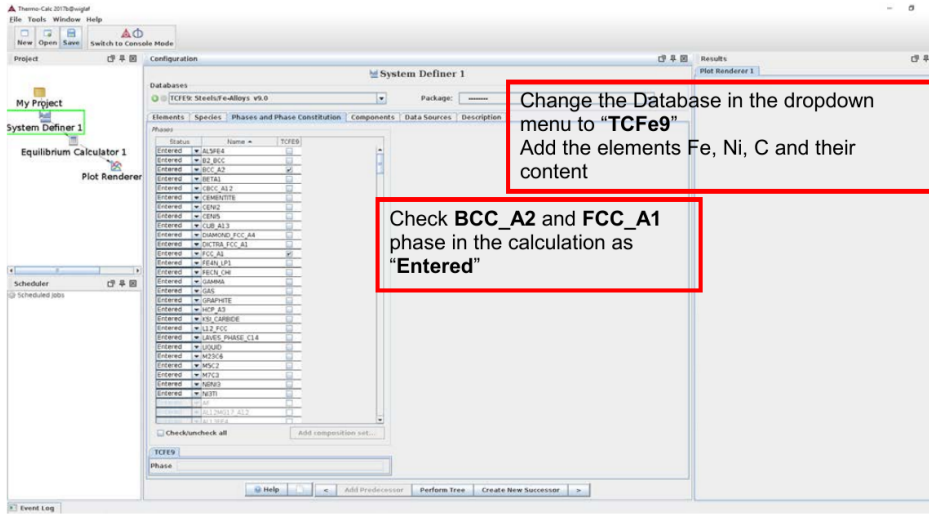
1. Open TC2021b and enter GUI mode. Select 'One Axis Equilibrium'



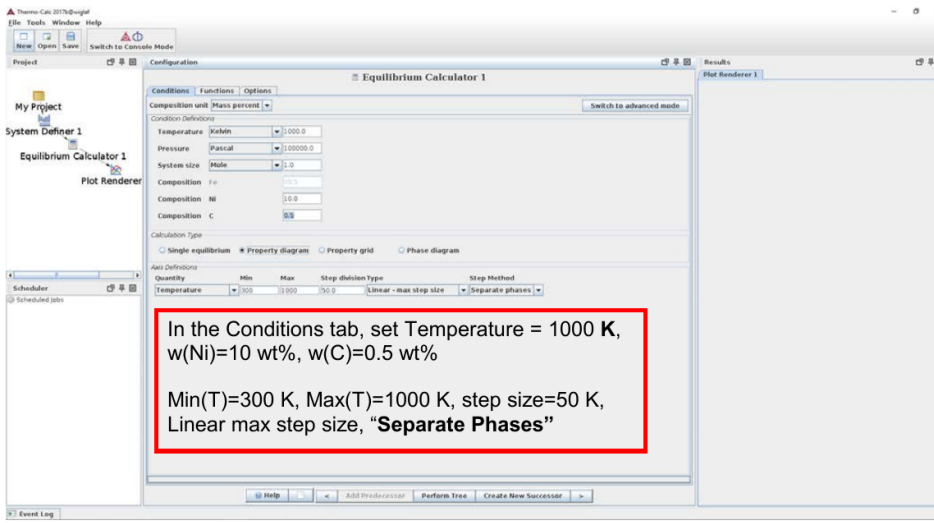
2. Change the database, add the correct elements, go to the Phases tab.



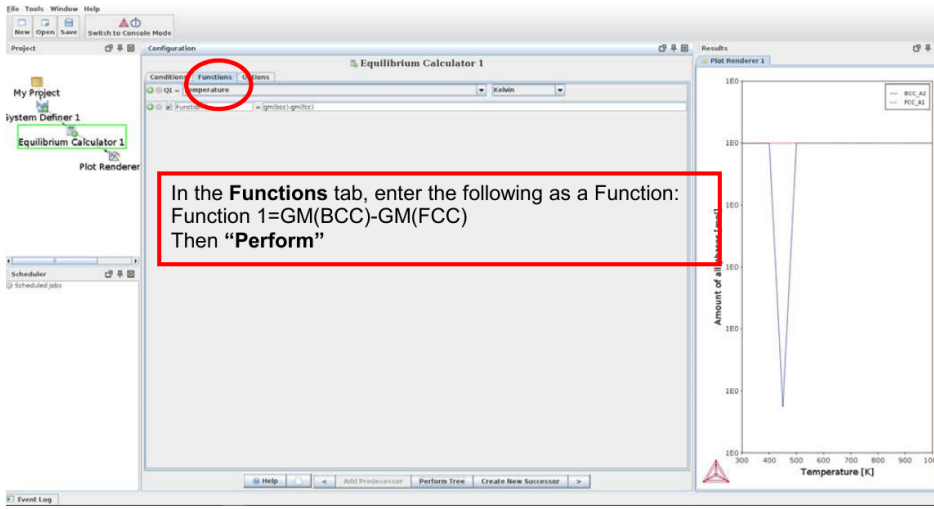
3. Choose Phases



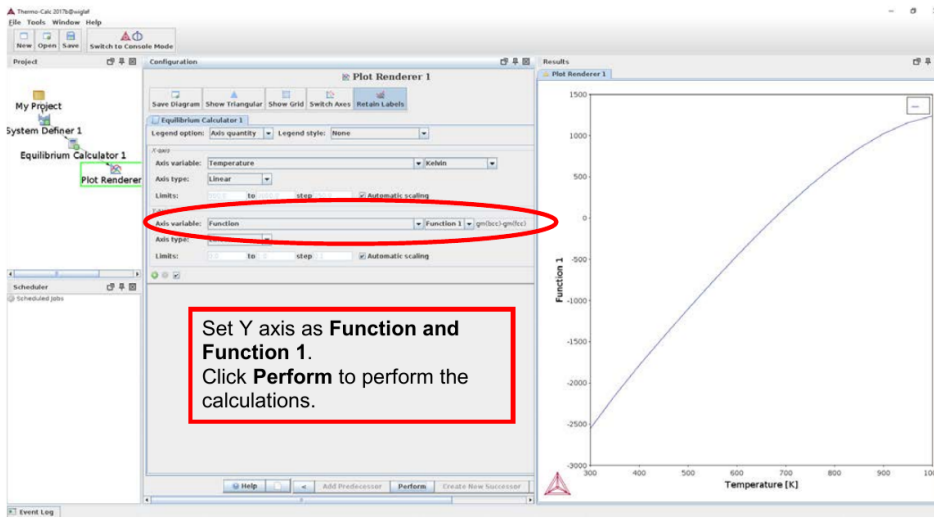
4. Set Conditions (Temperature and Composition).



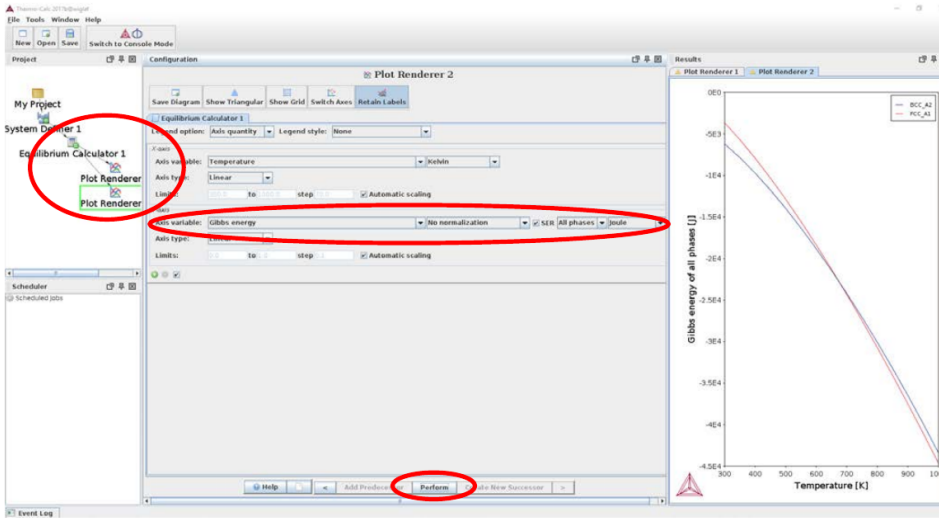
5. Enter Driving Force Functions



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?

8.3 Lab 3: DICTRA

8.3.1 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:

$$\frac{\partial C_k}{\partial t} = \nabla\left(D_k \nabla C_k\right), \tag{8.12}$$

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:

$$D_k = M_k C_k \frac{\partial \mu_k}{\partial C_k} \tag{8.13}$$

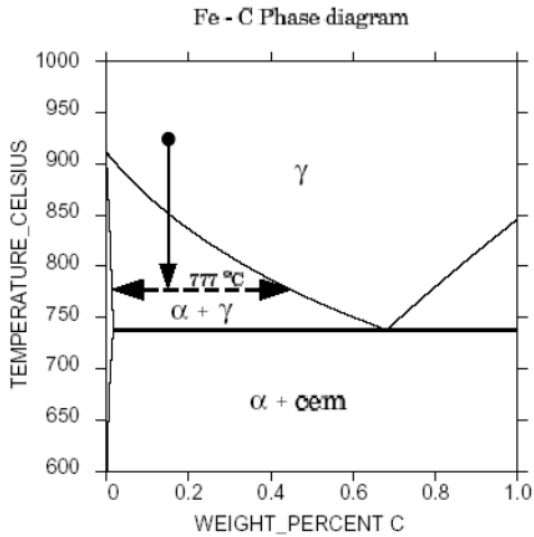
where μ_k is the chemical potential of component k. (See the 316-1 text for a more detailed description). Combination of Eqs. 8.12 and 8.13 gives:

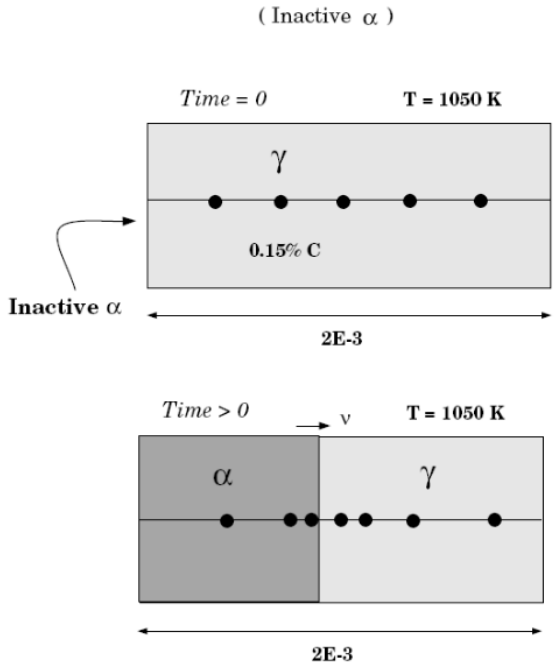
$$\frac{\partial C_k}{\partial t} = \nabla \left(C_k M_k \nabla \mu_k \right), \tag{8.14}$$

The diffusion database holds the mobility terms and the chemical potentials are extracted from the thermodynamic database. DICTRA solves Eq. 8.14 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).

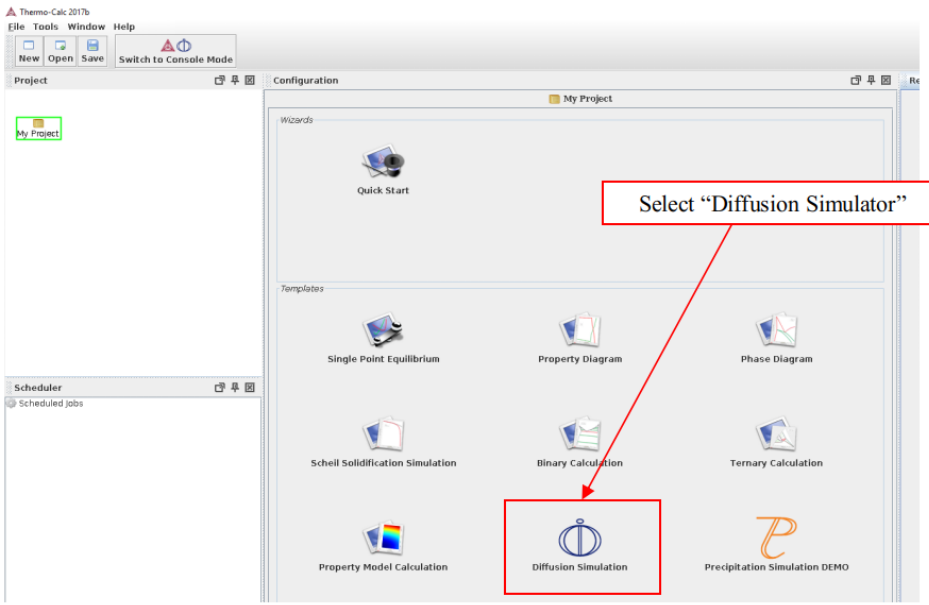
8.3.2 Example: γ to α transformation in a binary Fe-C alloy.

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:

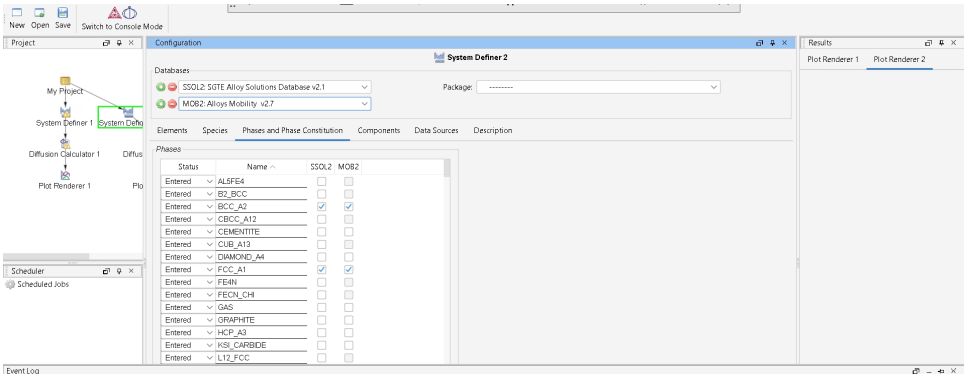


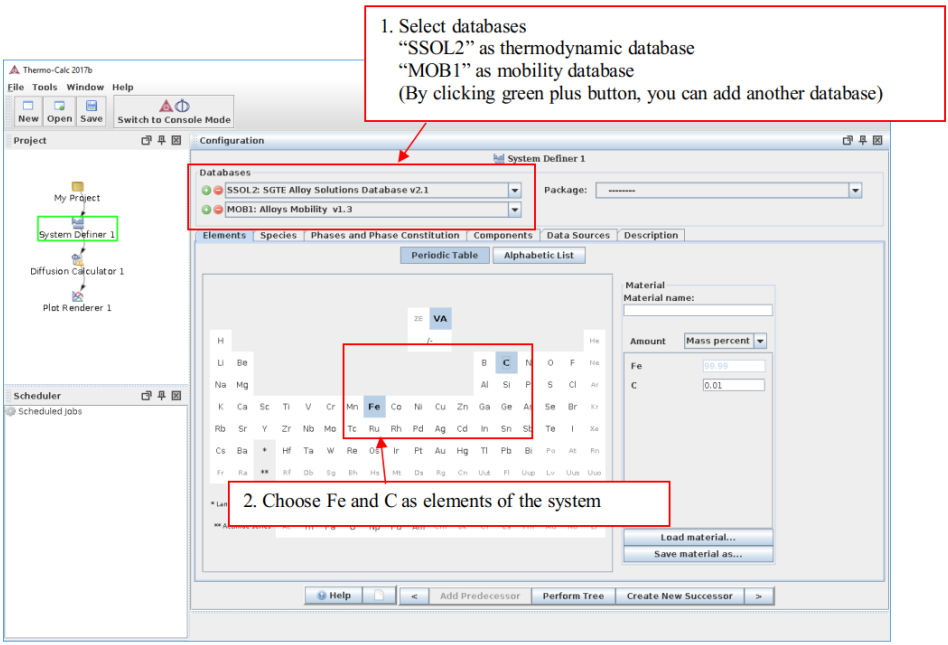


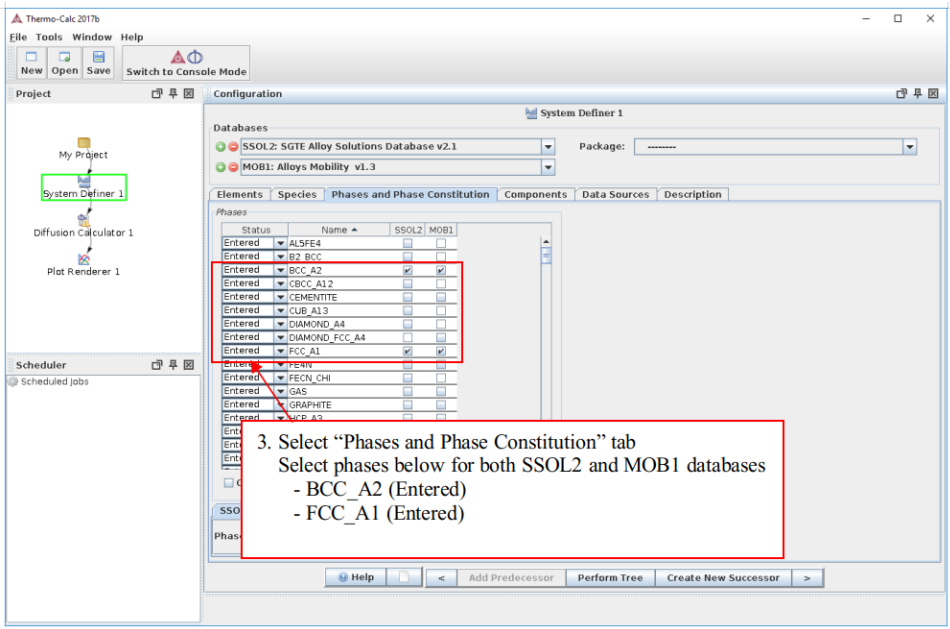
8.3.3 Step 1: Open Thermo-Calc 2021b and select "Diffusion Simulation"



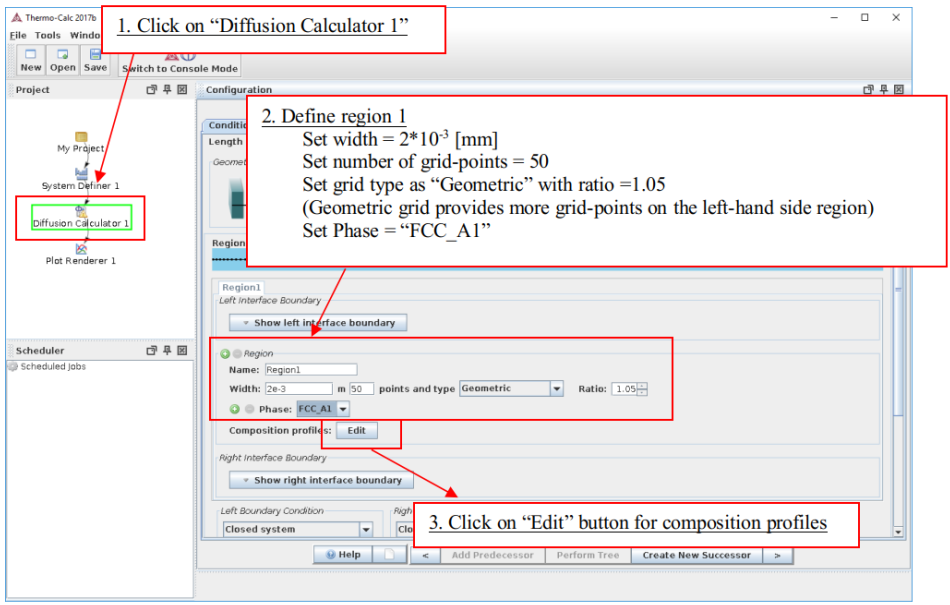
8.3.4 Step 2: Define The system: 1) Check "SSOL2" as the thermodynamic database, and "MOB1" as the mobility database.

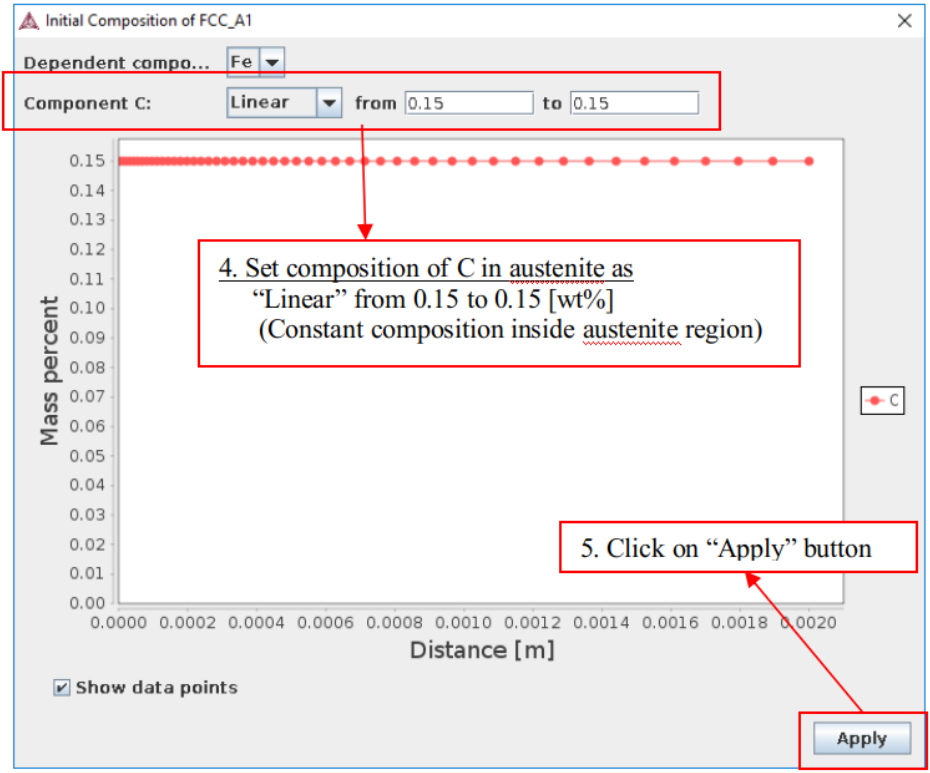


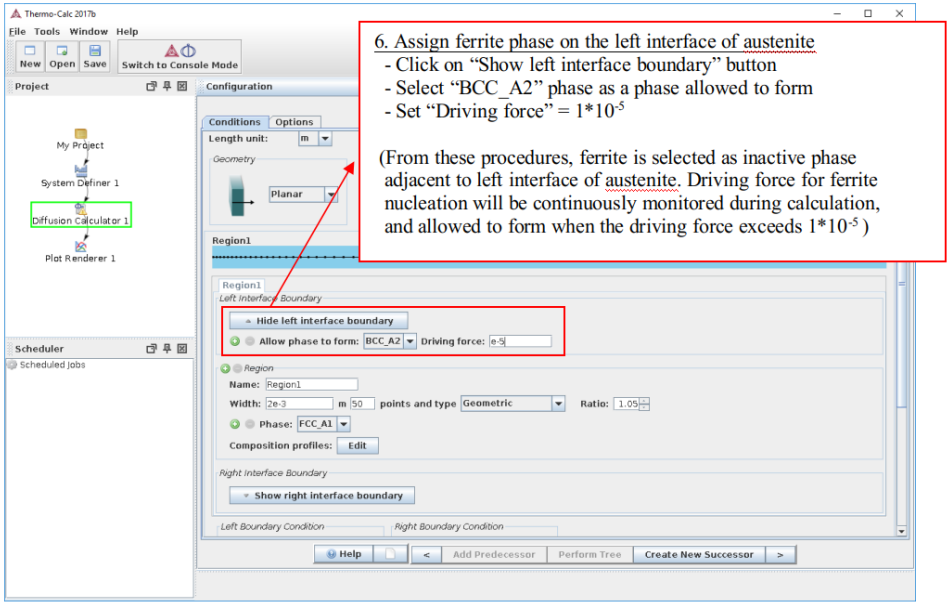


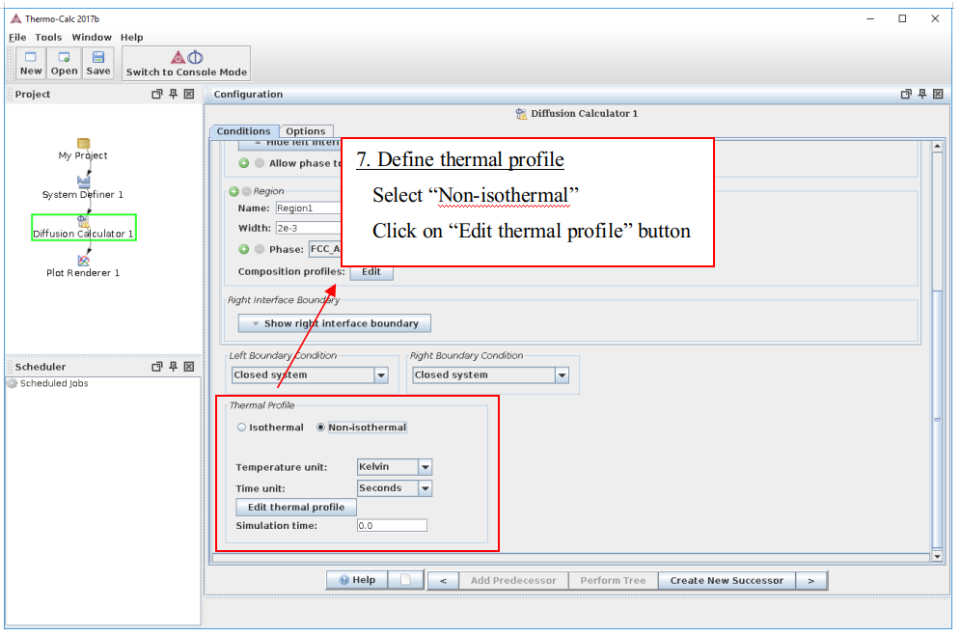


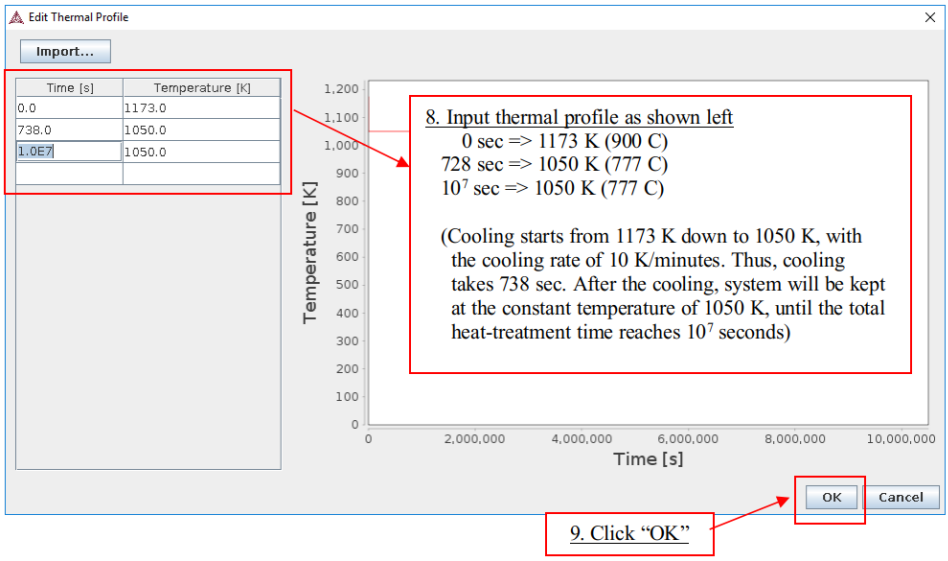
8.3.5 Define Calculation Conditions

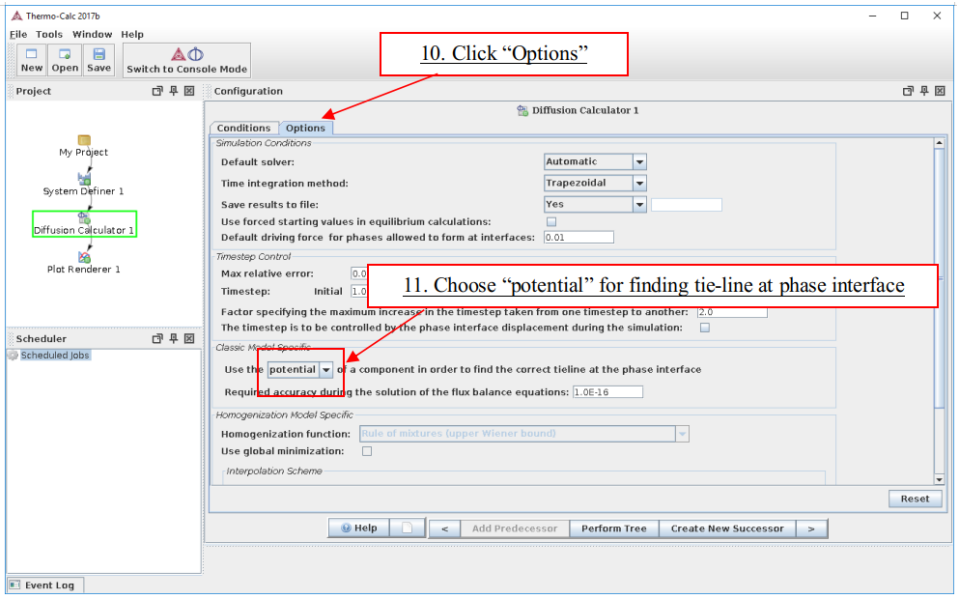



Initial Composition of FCC_A1
Dependent compo...
Fe
Component C:
Linear
from 0.15
to 0.15
4. Set composition of C in austenite as
"Linear" from 0.15 to 0.15 [wt%]
(Constant composition inside austenite region)
Mass percent
Distance [m]
C
5. Click on "Apply" button
Show data points
Apply

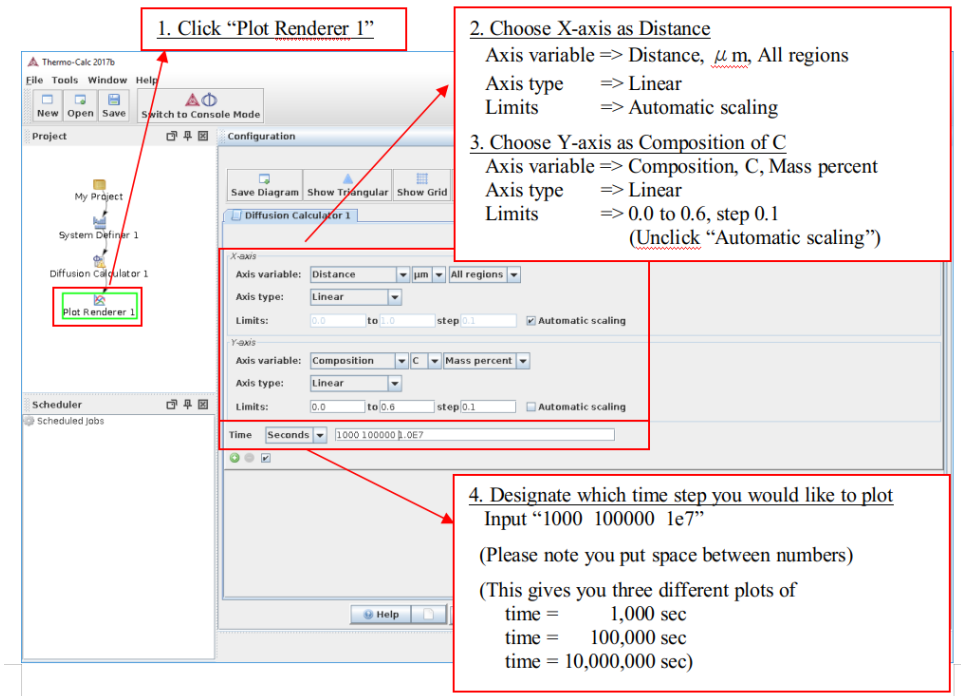

Thermo-Calc 2017b
File Tools Window Help
New Open Save
Switch to Console Mode
Project
Configuration
Conditions Options
Length unit:
Geometry
Planar
Region1
My Project
System Definer 1
Diffusion Calculator 1
Plot Renderer 1
Scheduler
Scheduled Jobs
Left Interface Boundary
Hide left interface boundary
Allow phase to form:
BCC_A2
Driving force:
Region
Name:
Width:
points and type
Geometric
Ratio:
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
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
Diffusion Calculator 1
My Project
System Definer 1
Diffusion Calculator 1
Plot Renderer 1
Conditions Options
7. Define thermal profile
Select "Non-isothermal"
Click on "Edit thermal profile" button
Region
Name: Region1
Width: 2e-3
Phase: FCC_A
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
Scheduler
Scheduled jobs
Help
Add Predecessor
Perform Tree
Create New Successor

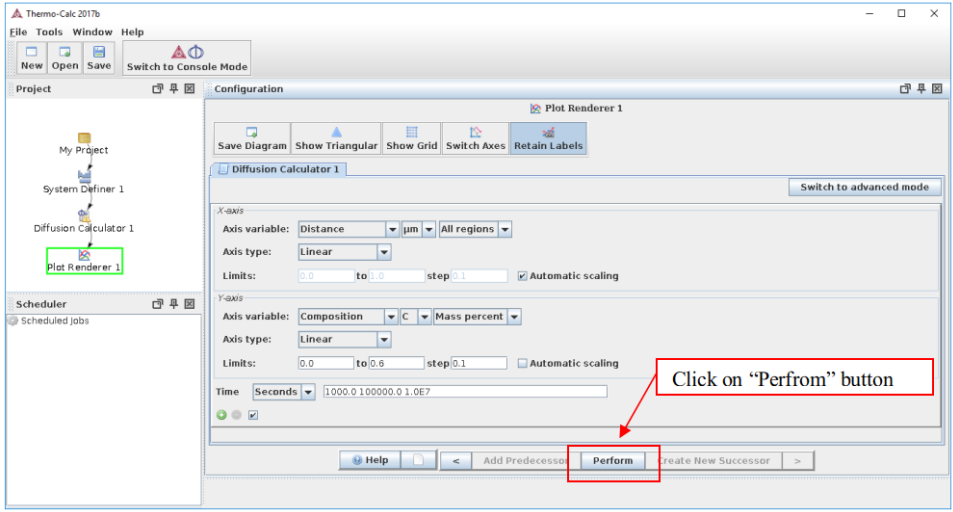

Edit Thermal Profile
Import...
Time [s]
Temperature [K]
0.0
1173.0
738.0
1050.0
1.0E7
1050.0
8. Input thermal profile as shown left
0 sec => 1173 K (900 C)
728 sec => 1050 K (777 C)
10^7 sec => 1050 K (777 C)
(Cooling starts from 1173 K down to 1050 K, with the cooling rate of 10 K/minutes. Thus, cooling 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)
Temperature [K]
Time [s]
OK
Cancel
9. Click "OK"



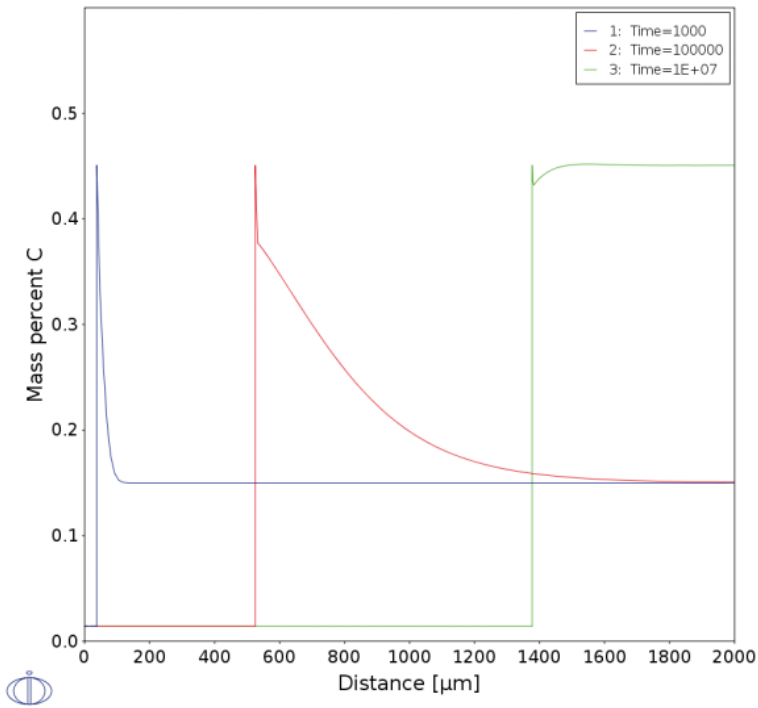
8.3.6 Step 4: Define Plot Conditions



8.3.7 Step 5: Execute Calculation



8.3.8 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.

8.4 Lab 4: PrecipiCalc/TC-PRISMA

8.4.1 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

8.4.2 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)

8.4.3 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

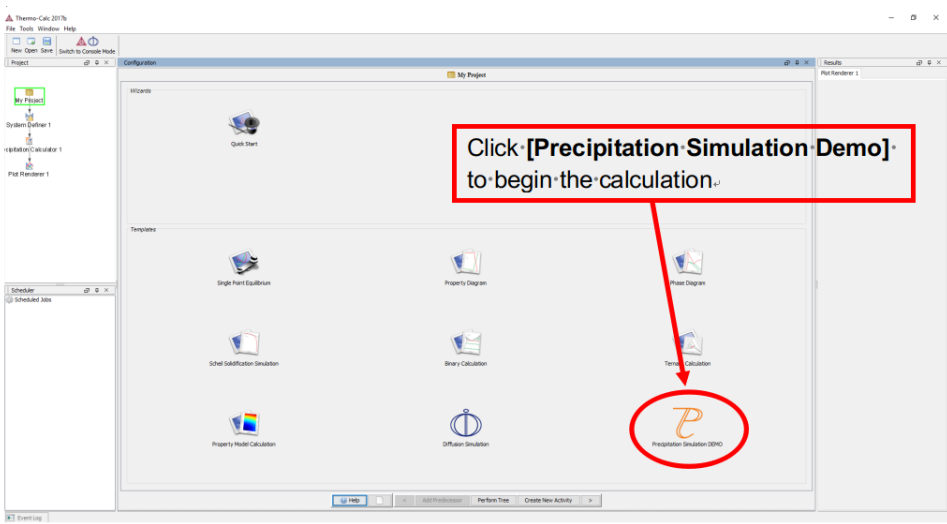
- ◇ Temporal evolution of particle size distribution
- ◇ Average particle radius and number density
- ◇ Volume fraction and composition of precipitate
- ◇ Nucleation rate and coarsening rate
- ◇ Isothermal transformation/Time-Temperature-Transformation (TTT) diagrams
- ◇ Continuous-Cooling-Transformation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

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

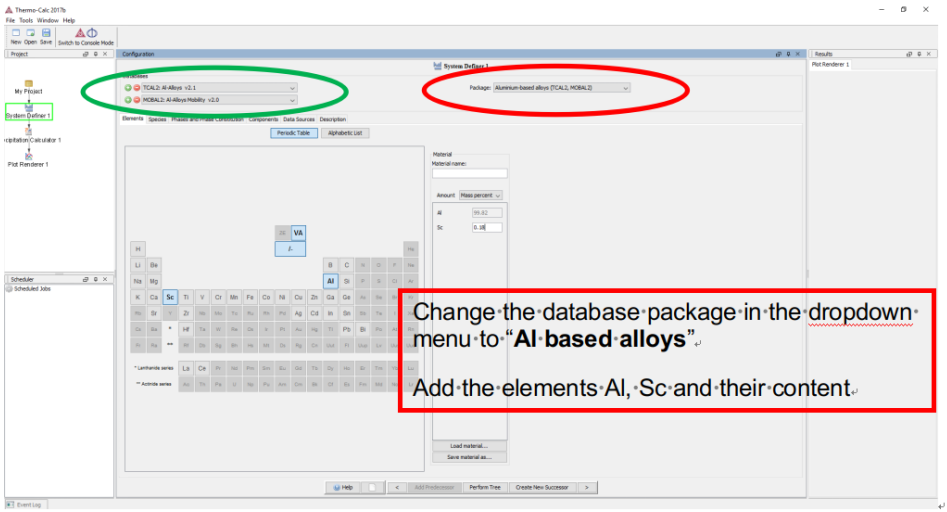
8.4.5 Example 1. Isothermal Precipitation of Al_3Sc in Al-0.18Sc (wt%) binary alloy

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

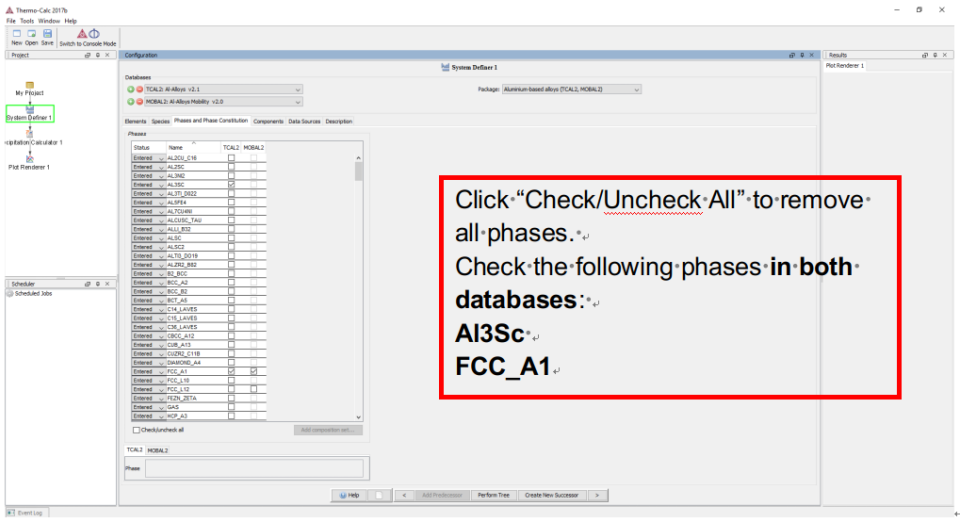
Step 1: Open TC2021b and enter GUI. Select 'TC-PRISMA'



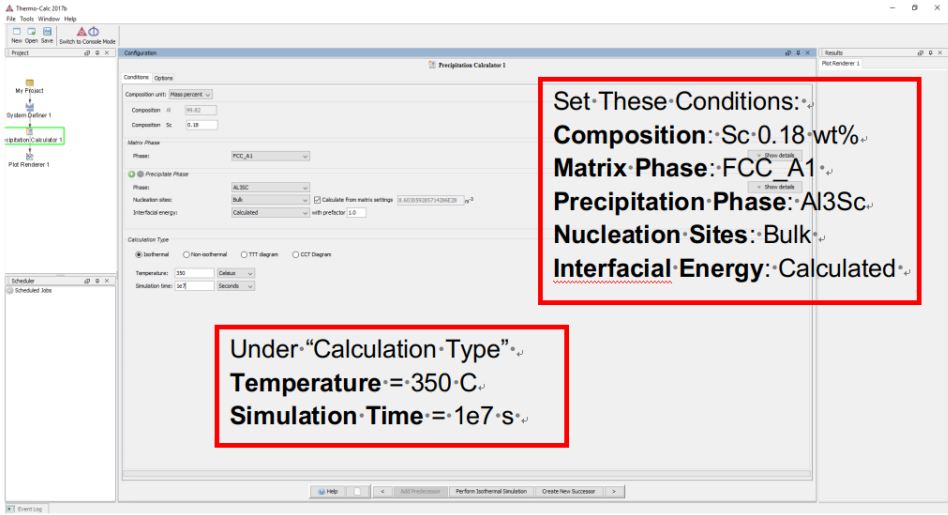
Step 2: Pick Database and Elements in System



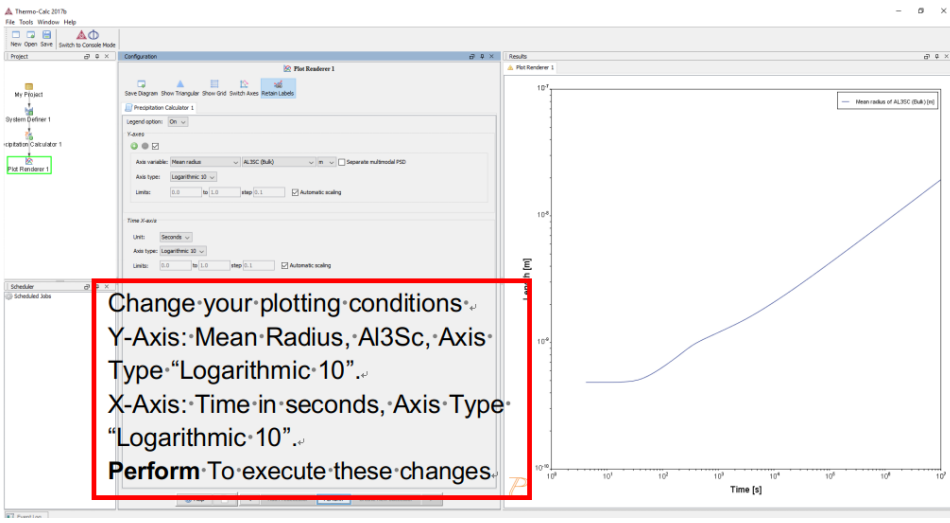
Step 3: Identify Phases in System



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

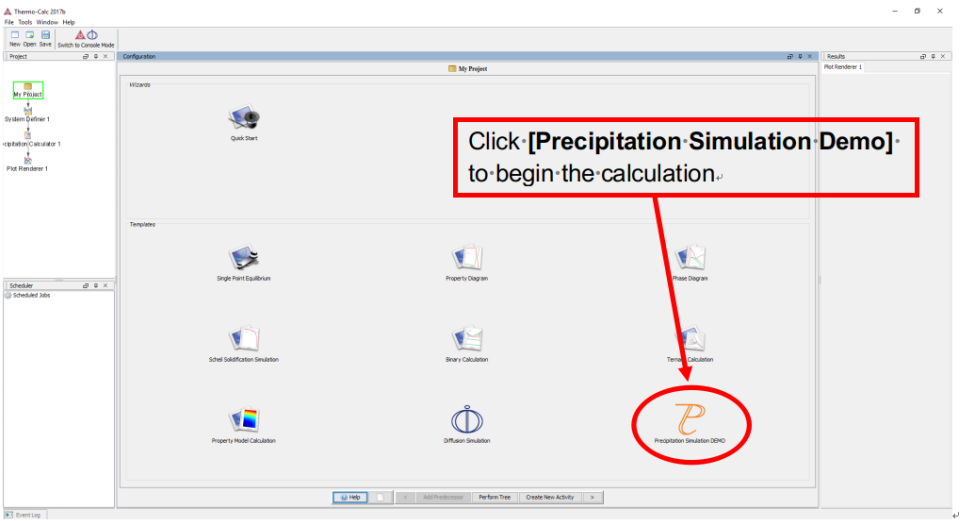


Step 5: Plot Renderer Results

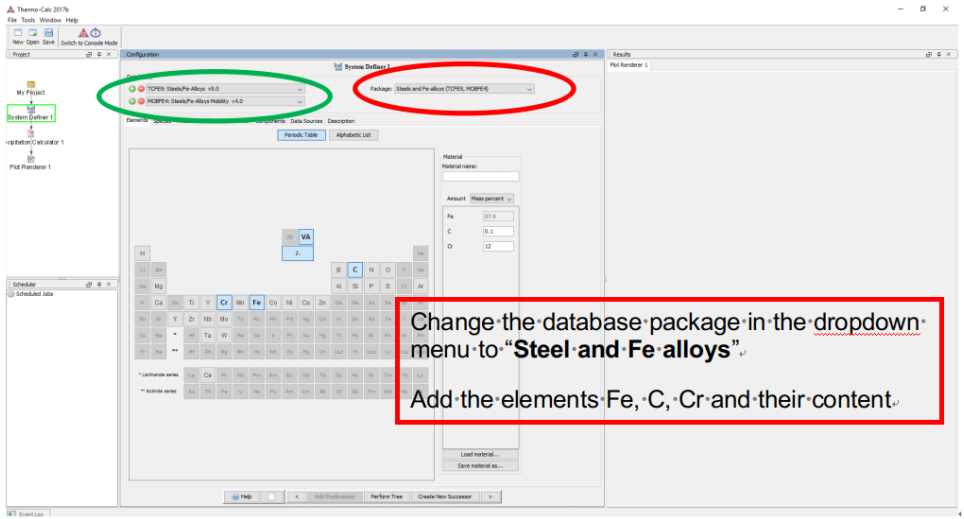


8.4.6 Example 2. Stable and Metastable Carbides in Fe-0.1C-12Cr (wt%) Steel - TTT Diagram

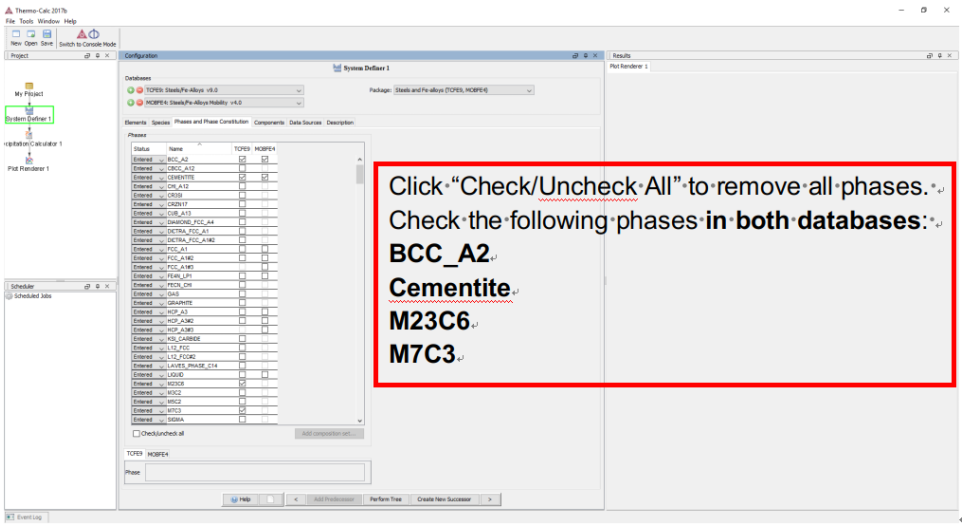
Step 1: Open TC2021b and enter GUI. Select 'TC-PRISMA'



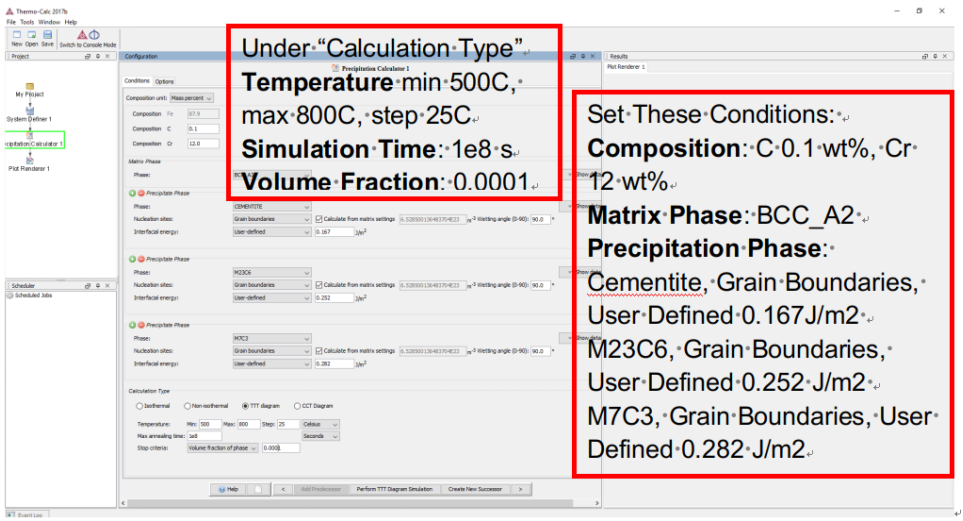
Step 2: Pick Database and Elements in System



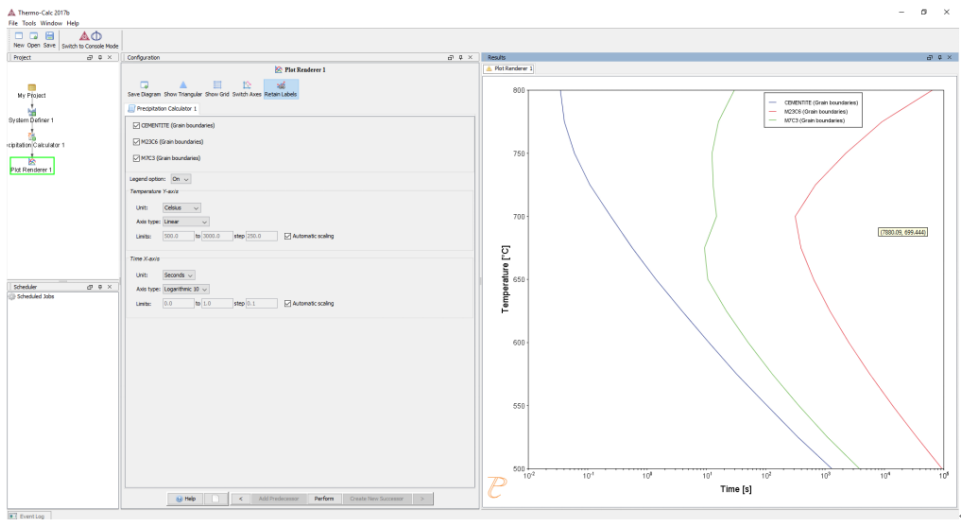
Step 3: Identify Phases in System



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



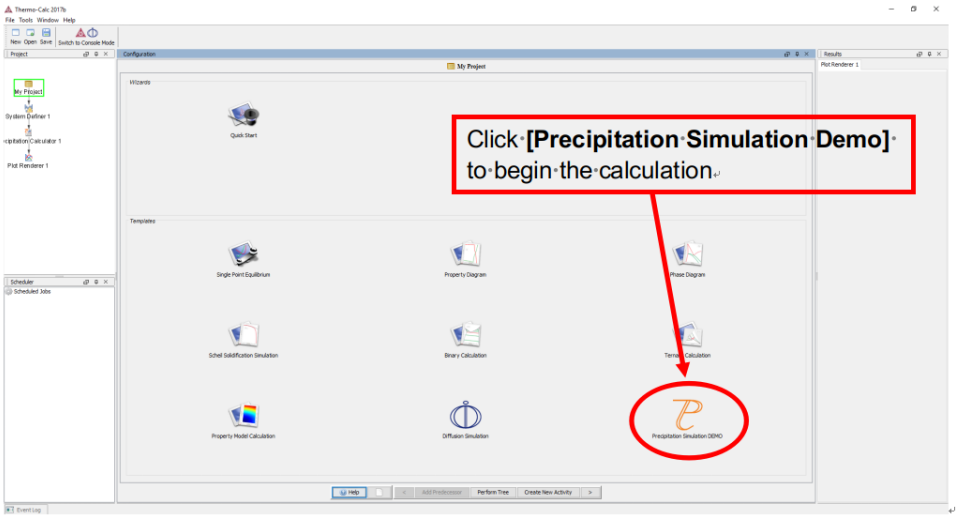
Step 5: Plot Renderer Results



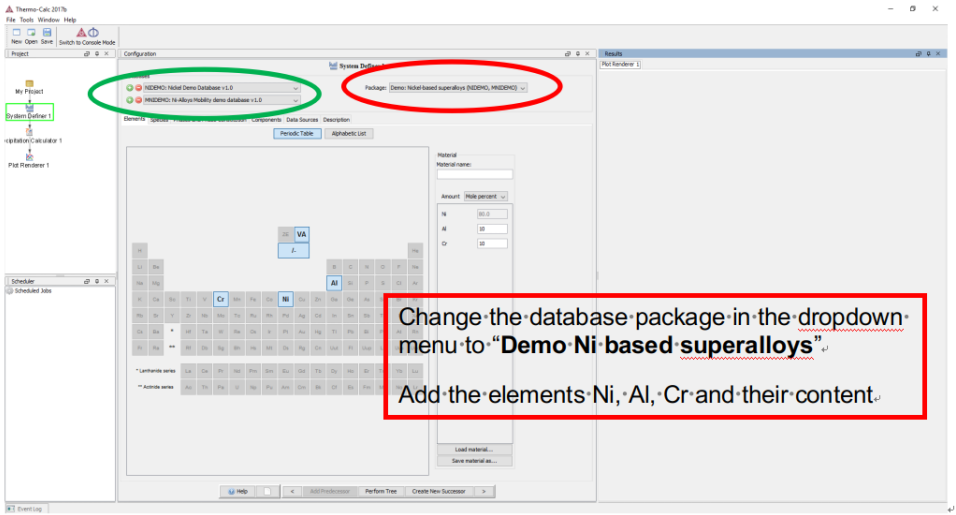
8.4.7 Example 3. Cooling Rate Diagram of $\gamma - \gamma'$ Ni-10Al-10Cr (at%) superalloy – CCT diagram

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.

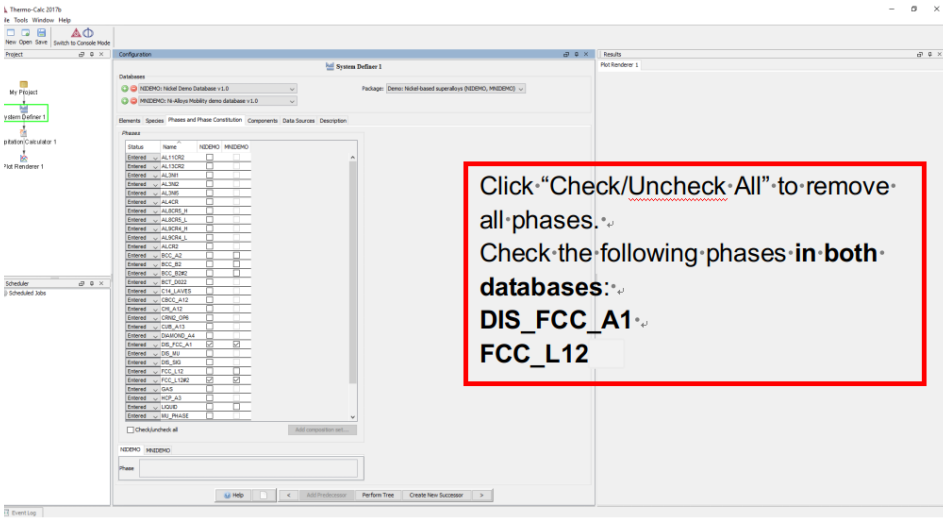
Step 1: Open TC2021b and enter GUI. Select 'TC-PRISMA'



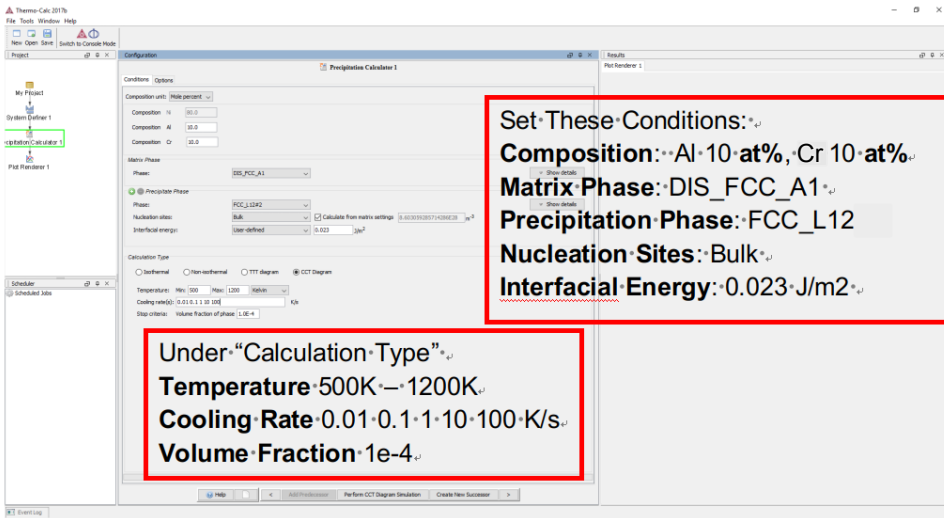
Step 2: Pick Database and Elements in System



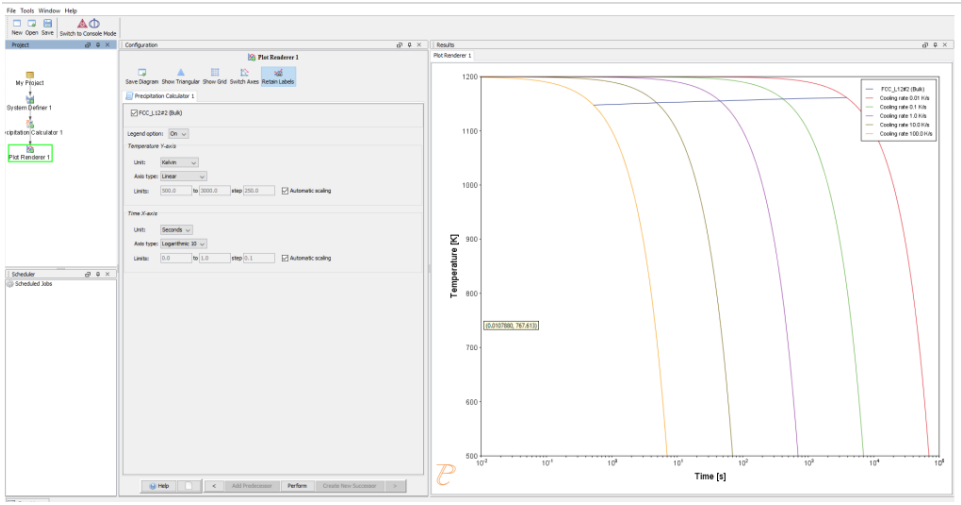
Step 3: Identify Phases in System

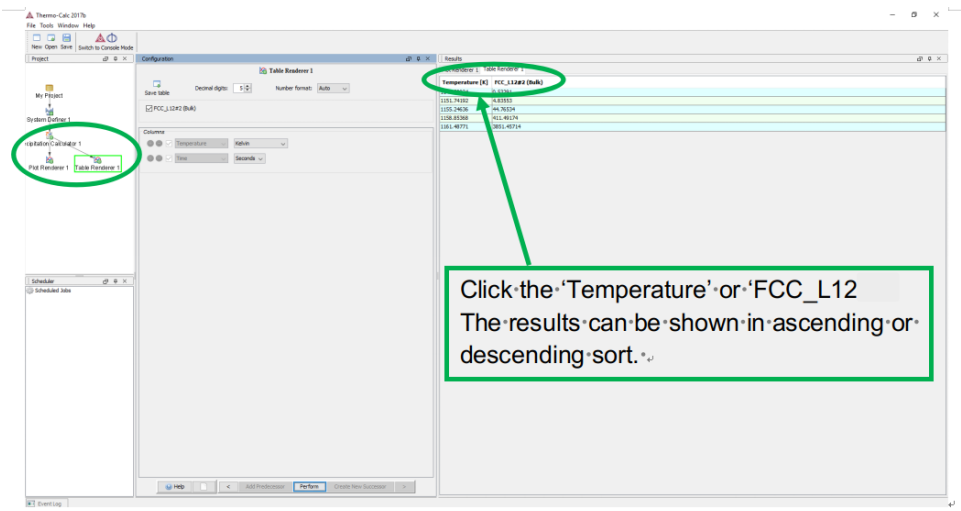


Step 4: Set Simulation Conditions for CCT diagram. Then Perform calculation. The calculation would take a few minutes.



Step 5: Plot/Table Renderer Results





9 390 Homeworks

9.1 Materials Selection in Mechanical Design

In order to receive credit for the CES materials selection problems, you must:

- ◇ answer the questions
- ◇ explain the process used to get your answers
- ◇ include ALL relevant CES plots with explanations of the information given on each plot in all problems. CES plots should be properly enlarged in specific regions if needed, and failed records of materials (materials that do not satisfy the criteria shown in gray) should be hidden.

There is no unique answer to the questions. Therefore, your grade will not be determined by the particular materials you choose. You can select any materials

that satisfy the criteria and as long as you explain the process used to get your answer.

Start from "Level 3" database and "All bulk materials" for all problems.

To change units go to: tools → settings → units → <automatic-metric> or <metric>

1) General use of the CES database: Answer the following using CES database:

(a) A component is currently made of soft commercially pure Gold. Due to high cost of gold, please use CES to suggest two other materials that have greater thermal conductivity.

(b) Find a material with $250 < E < 350$ GPa and density $7,000 < \rho < 8,000$ kg/m^3.

(c) Which have higher specific stiffness, E/ρ : titanium alloys or tungsten carbides?

(Hint: use 'Tree' in the selection stage to select titanium alloys and tungsten carbides only)

(d) Is the fracture toughness, K_{IC}, of common engineering polymers like PVC elastomer (Shore A60) higher or lower than those of engineering ceramics like silicon carbide (HIP)?

2) Multi-stage materials selection using CES database You are employed by a company that manufactures various sports goods except tennis rackets. Even though the company is doing well, in an effort to expand company's market the management decided to introduce a new product: tennis rackets. Being the only Materials Engineer in the company your new assignment is to select four different materials that would be suitable for manufacturing tennis rackets.

Since you have already used CES, you should not have any problem in getting started. First, let us examine the essential functions of a body of a tennis racket: structural support for the string, transfer of force, absorption of energy (damping) etc. Often, the tennis rackets are also subjected to mechanical abuse (due to bad temper or frustration of the players). Thus, the optimal materials must be light, stiff, strong, and should have reasonably good fracture toughness. In conjunction with the CES database, the following multi-stage criteria may be applied to select off-the-shelf materials suitable for manufacturing tennis rackets.

Stage I: Assume that due to the complex shape of the body of the tennis racket the maximum stiffness at minimum weight is given by the following performance index:

$$M_1 = \frac{\sqrt{E}}{\rho} \tag{9.1}$$

where E is the Young's Modulus, and ρ is the density.

Stage II: The maximum ductile strength of rods at minimum weight is given by the following performance index:

$$M_2 = \frac{\sigma_y^{0.8}}{\rho} \tag{9.2}$$

where σ_y is the yield stress (Elastic Limit in CES).

Stage III: The maximum fracture toughness of rods at minimum weight is given by the following performance index:

$$M_3 = \frac{K_{IC}}{\rho} \tag{9.3}$$

where K_{IC} is the fracture toughness.

Stage IV: Selection of materials that will give minimum density and maximum damping capacity. In CES, the damping behavior is represented by the Mechanical Loss Coefficient under Optical, aesthetic and acoustic properties. A higher mechanical loss coefficient implies a better damping capacity. Use Box Method for selecting a subset of materials (with $\rho < 2{,}000$ kg/m3 and mechanical loss coefficient greater than 0.008) in this stage.

Use the above four stages of selection to determine the optimal materials for tennis racquets. The materials must also satisfy the following:

- $M_1 > (10^3\,\text{Pa})^{0.5}/(\text{kg/m}^3)$
- $M_2 > (10^4\,\text{Pa})^{0.8}/(\text{kg/m}^3)$
- $\text{M}_3 > (10^4\,\text{Pa}\sqrt{\text{m}})/(\text{kg/m}^3)$

(See the note in section 8.1 to better understand how to interpret these values of the performance index).

Turn in the following:

(a) Graphical output for each stage showing the selection line/box. In the report, you must explain how you have drawn the selection line in each stage;

(b) Table for Materials passing 4 of the 4 stages

(c) Select four different materials that passed all the stages for manufacturing tennis rackets. At this stage you may consider cost (listed in CES) so that rackets will have a wide range of price. List the Young's modulus, the yield stress, the fracture toughness, the loss coefficient, and price of the materials you selected, in a table like the one outlined below:

Material	E (Pa)	σ_y (Pa)	K_{IC} (MPa$\sqrt{\text{m}}$)	Mech. Loss Coeff.	Price

3) Multi-stage materials selection using CES database: As an engineer at a minor aircraft company, you have been given the task of determining the proper material for use as an aircraft door. After research you have determined nine properties that the material must possess. They are as follow:

- ◇ Fracture toughness, $K_{IC} > 40$ MPa$\sqrt{m}$
- ◇ Young's Modulus, $E > 100$ GPa
- ◇ Density, ρ 5,000 kg/m^3
- ◇ Thermal Expansion $< 20\text{x}10^{-6}/^{\circ}\text{C}$
- ◇ Elongation > 10 %
- ◇ Cost < 20 USD/kg
- ◇ Recycle fraction in current supply > 20 %
- ◇ Flammability = {non-flammable}
- ◇ Durability in fresh water = {excellent}

Determine a suitable material for this application

9.2 Thermo-Calc

Requirements for Thermo-Calc questions:

- ◇ Your answers to all of questions must be substantiated by calculated diagrams and I should be able to make out as to what you have to plot in the figure(s)
- ◇ Everyone must submit his/her own calculated diagram(s)
- ◇ The title of the phase diagrams MUST be your name
- ◇ All phase fields must be labeled; and (v) a copy of the equilibrium results obtained from the TC 2017b window must accompany the answers that require equilibrium calculations
- ◇ You will receive an automatic zero if it is found that you have submitted someone else's phase diagram or graph.
- ◇ **Warning:** The phase labeling function of TC2017b occasionally gives you obviously wrong results. You may try removing all labels and adding them again, or adjusting window/graph sizes. If you can't get it right from the software, clarify the situation and give your answers in your homework.

4) Pb-Sn solders are widely used in electronic packaging (chip-to-chip and chip-to-carrier interconnections) and various other applications related to soldering. However, due to toxicity of Pb and environmental concerns, Pb-Sn solders have been banned in many applications, such as, food packaging (e.g., beverage cans), certain plumbing applications etc. The Sn-In phase diagram is important for designing multicomponent Pb-free solders.

Hints: (i) Use SSOL2 database; (ii) For both the Pb-Sn and In-Sn systems, consider the following phases only: LIQUID, FCC_A1 and BCT_A5; (iii) temperature limits for mapping: 0 – 400°C for both alloys. In the SSOL database, the Sn-phase is defined by BCT_A5, because its structure is body centered tetragonal, the In-phase and Pb-phase are defined by FCC_A1, because both of their structures are face centered cubic.

(a) Calculate Pb-Sn and In-Sn equilibrium phase diagrams. You have to submit the calculated phase diagrams with all phase fields labeled.

(b) What are the calculated eutectic temperatures in Pb-Sn and In-Sn systems?

(c) What are the calculated solid solubilities of Pb in Sn and In in Sn at their respective eutectic temperatures? Answer this question both in weight and atomic percents of Pb and In.

(d) Despite toxicity/environmental concerns, Pb-Sn solders are widely used in all microelectronic packages. In particular, the Pb-Sn eutectic alloy. For a Sn-38 wt.% Pb alloy, answer the following:

i What are the phases present at 50 $^\circ$ C and 130 $^\circ$ C? (Note: many devices, such as computers operate in this temperature range)

ii What are the amounts and composition (in wt%) of the phases present at 50 and 130 $^\circ$ C?

iii What are the important differences you notice between the calculated results at these two temperatures?

5) Calculation of the Ms temperature (temperature when martensite starts to form) is a very crucial step in designing ultra-high strength, secondary hardening martensitic steels. Such a calculation allows us to select the alloy(s) whose Ms is sufficiently high so that upon quenching (from solution treatment temperature) to room temperature a fully martensitic microstructure is obtained. If the Ms is not high enough, then we may get incomplete transformation at room temperature and the alloy will need to be quenched at sub-ambient temperatures. Therefore, an alloy with an Ms>300°C would be desirable.

Hints: (i) Use the SSOL2 database; (ii) consider the following phases for 2.1-2.4: BCC_A2 and FCC_A1, consider the following phases for 2.5: LIQUID, BCC_A2,

FCC_A1, HCP_A3, SIGMA, CEMENTITE, M23C6, and M7C3 (iii) stepping ranges for 2.1-2.4: 200 to 1000°C for temperature; mapping ranges for 2.5: 750 to 1250°C for temperature (iv) A solution treatment temperature is defined as the temperature at which all solutes will be in solid solution in one phase.

The alloy is based on iron with different concentrations of C, and with 14 wt. % Co, 8 wt. % Cr , 6 wt% Ni, 0.5 wt. % Mo and 0.3 wt. % V.

(a) What is the T0 temperature of the above alloy as a function of C content? Consider carbon concentrations 0.1 wt%, 0.3 wt%, 0.5 wt%, 0.7wt% and 0.9 wt%?

(b) Comment of the effect of C on the T0 temperature.

(c) Assuming that the martensitic transformation starts at a Driving Force of -1500 J/mol, what is the Ms temperature of the above alloy as a function of C content at 0.1 wt%, 0.3 wt%, 0.5 wt%, 0.7wt% and 0.9 wt%?

(d) Comment on the compositional dependence of Ms temperatures and determine which alloy(s) would be appropriate for the application stated in the above question.

(e) Calculate the vertical section of this alloy. For a solution treatment temperature of 1000°C, what is the maximum amount of C that can be put in the alloy? Show this point of the phase diagram.

9.3 DICTRA

To receive credit:

- ◇ Your answers to all of questions must be substantiated by calculated diagrams or table renderer results
- ◇ everyone must submit his/her own calculated diagram(s)
- ◇ the title of the phase diagrams MUST be your name

6) γ to α transformation in a ternary Fe-0.15wt%C-0.50wt%Si steel, when cooled from 1173K down to 1050K with the cooling rate of 10K/minute, and then isothermally held at 1050K until total heat-treatment time reaches 107 sec.

(a) Provide a plot of carbon concentration vs distance at t=1,000, 100,000, 10^7 sec.

(b) Provide a plot of silicon concentration vs distance at t=1000, 100000, 107 sec. Compare with the plot of the carbon concentration. Which element do you think is more mobile in this steel at this temperature, C or Si?

Hints:

- ◇ Use the SSOL2 database as thermodynamics database, and MOB1 database as mobility database
- ◇ Consider the following phases: FCC_A1 (γ, austenite) and BCC_A2 (α, ferrite)
- ◇ assume fully homogenized austenite (FCC_A1) at the beginning of the heat-treatment
- ◇ apply 50 grid-points of geometric grid with ratio = 1.05 in the initial austenite region
- ◇ assume ferrite starts to form when the driving force exceeds 10-5 (vi) use potential (not activity) for finding tie-line at the phase interface

9.4 TC-PRISMA

To receive credit:

- ◇ Your answers to all of questions must be substantiated by calculated diagrams or table renderer results
- ◇ everyone must submit his/her own calculated diagram(s)
- ◇ the title of the phase diagrams MUST be your name

9.4.1

Isothermal precipitation calculation of *gamma*-γ' Ni-12Al (at%) alloy at 450 °C for 1e15 s

Hints:

- ◇ Use the Demo Ni alloys database package
- ◇ Consider the following phases: DIS_FCC_A1 (matrix) and FCC_L12 (precipitate)
- ◇ Precipitate nucleation sites: bulk, interfacial energy 0.035 J/m2

(a) What is the maximum number density of precipitate? How long does it take to reach the maximum number density of precipitates (in hours)?

(b) What is the volume fraction of precipitate phase and matrix composition (Al concentration in at%) at 1e15 s?

9.4.2

3. Isothermal precipitation calculation of metastable and stable carbides in Fe-0.1C-12Cr (wt%) at 750 °C for 1e6 s

(a) From the volume fraction vs. time figure, can you tell the sequence of precipitation?

Hints:

- ◇ Use the Steel and Fe alloys database package;
- ◇ consider the following phases: BCC_A2 (matrix), CEMENTITE (precipitate), M23C6 (precipitate), and M7C3 (precipitate)
- ◇ precipitate nucleation sites: grain boundaries
- ◇ interfacial energy: CEMENTITE (0.167 J/m^2), M23C6 (0.252 J/m^2), M7C3 (0.282 J/m^2)
- ◇ plot volume fraction of all three carbides (linear) vs. time (log 10)

(b) Can you obtain this precipitation sequence without doing this isothermal calculation?

Hint:

Example 2 in Lab 5b tutorial

(c) What the volume fraction of the stable precipitate phase at 10^6 s? How about its equilibrium volume fraction?

Hint:

TC single point equilibrium calculation using TCFE9 database with BCC_A2, CEMENTITE, M23C6, and M7C3 entered