CME-572: HW5/Final Project Report

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[redacted]

Project Name: Final Project – CME 572: Advanced Thermodynamics of Materials

Project Semester: Spring 2024

Submitted to Prof. Sara Kadkhodaei

Project Details

Material Selected	Motivation	Software Used
Al-Mg	1. Al-Mg alloys find a broad range of applications in transport, construction, etc. 2. The Al-Mg phase diagram has enough complexity to be analyzed for this project	Thermo-Calc 2023a (Pro)-GUI Mode

Computing Resource Provided By: SEL 1258 UIC

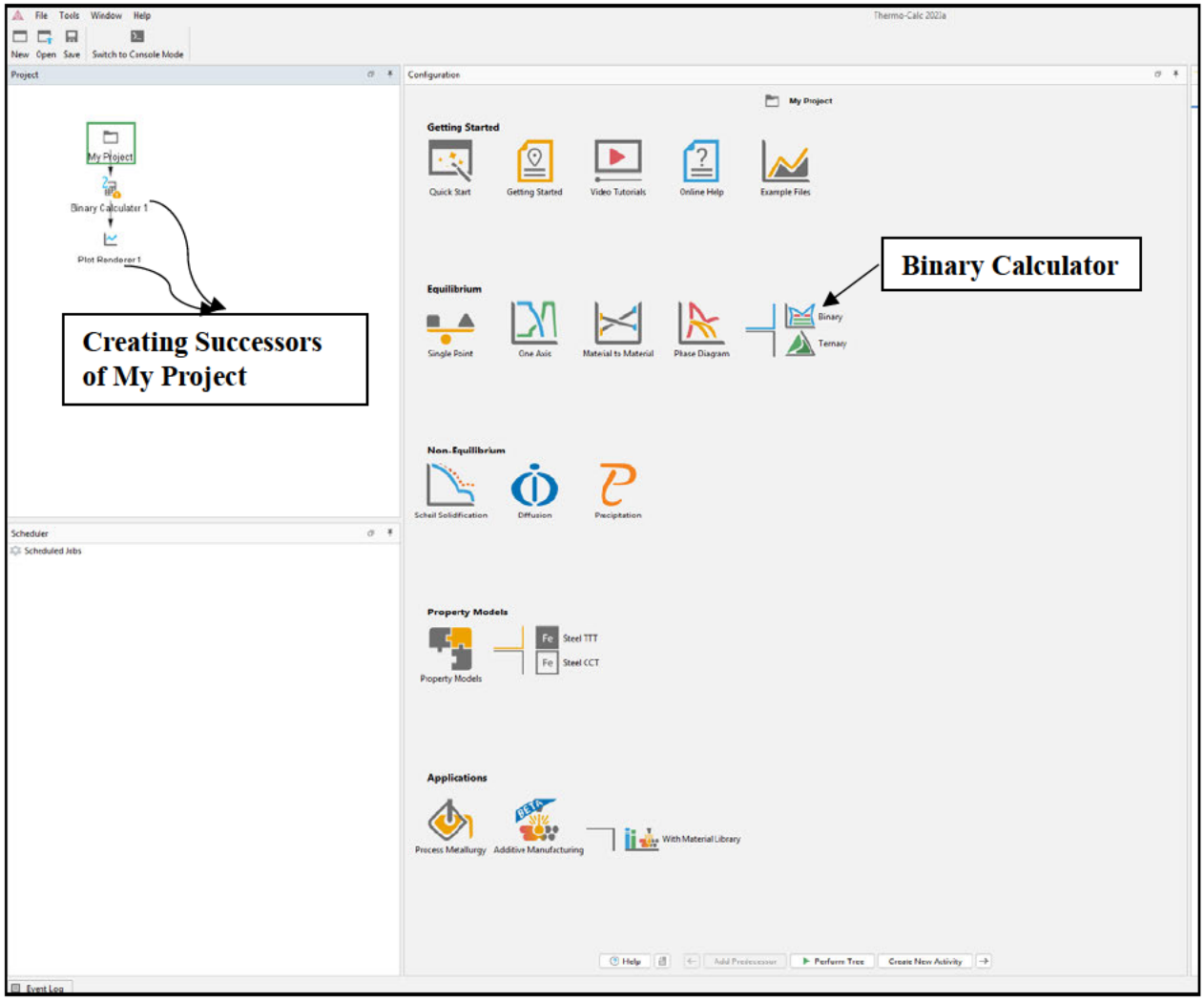
I. Calculation of the Phase Diagram

Assumptions:

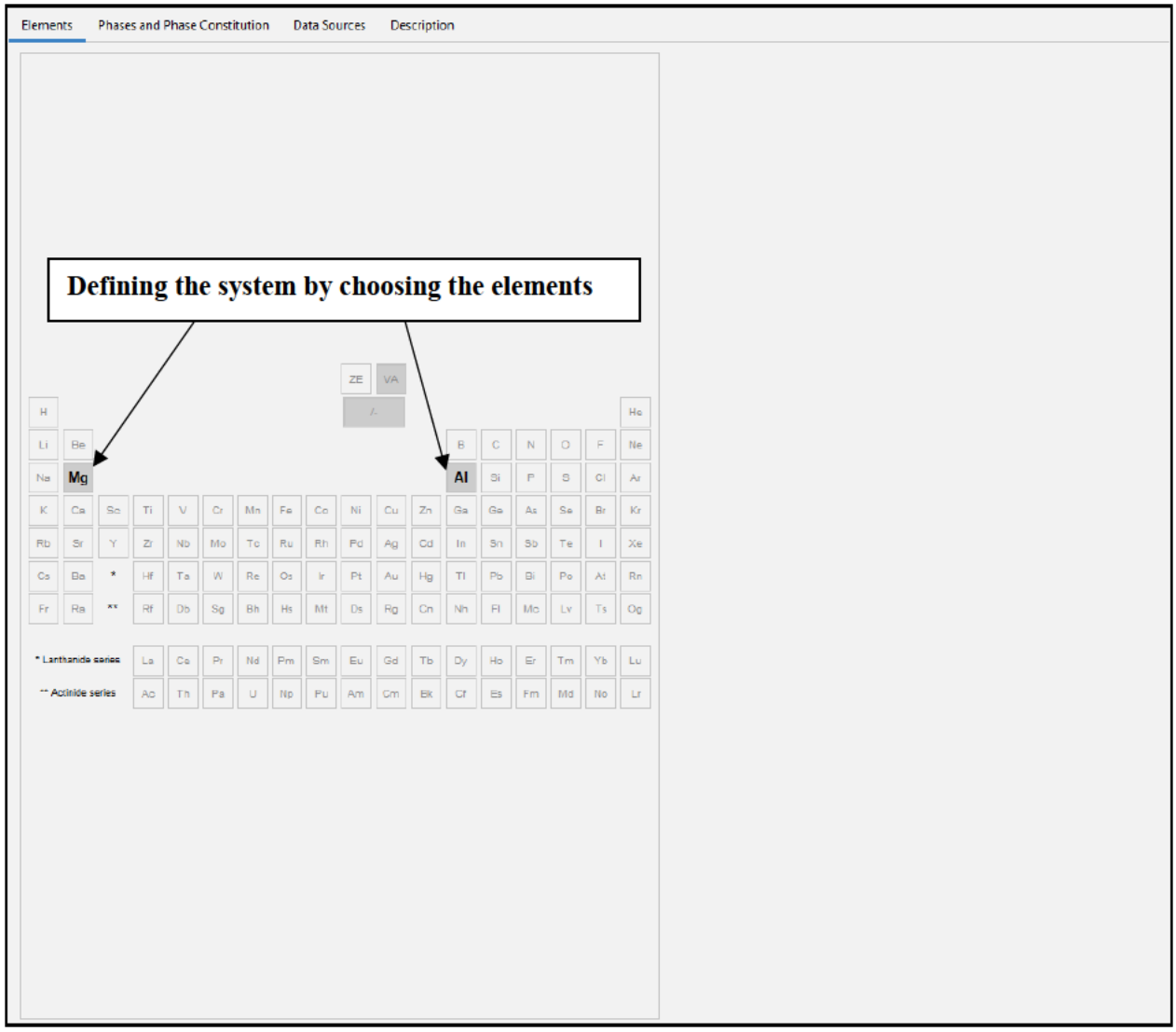
1. Selected temperature range for phase diagram construction: 298- TBU K
2. TCAL8: Al-alloys v8.2

(a) Stepwise illustration of the calculation process

1. Selection of binary calculator in My Project:



2. Defining the system:



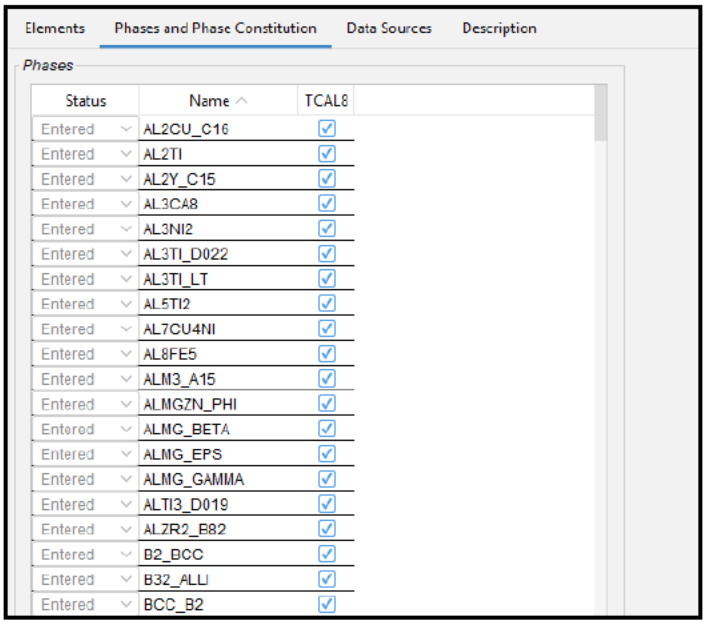
The above elements are selected out of the pool of available elements in the TCAL8: Al-alloys v8.2 for the current system which is the Al-Mg alloy.

For the binary calculation, the maximum allowable elements are two which can be selected in any order.

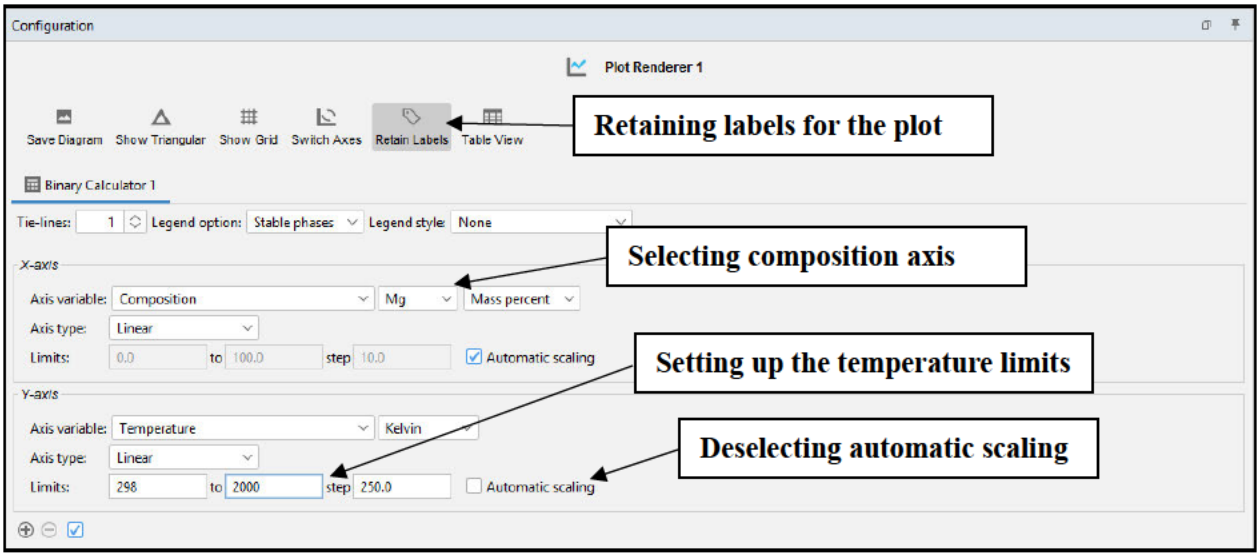
3. Setting up the phase diagram calculation:

4. Choosing additional settings:

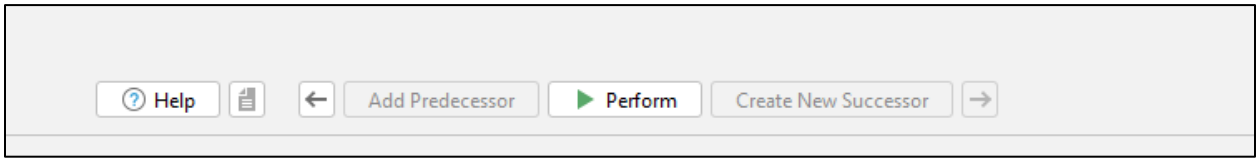
i) Phases and phase constitution

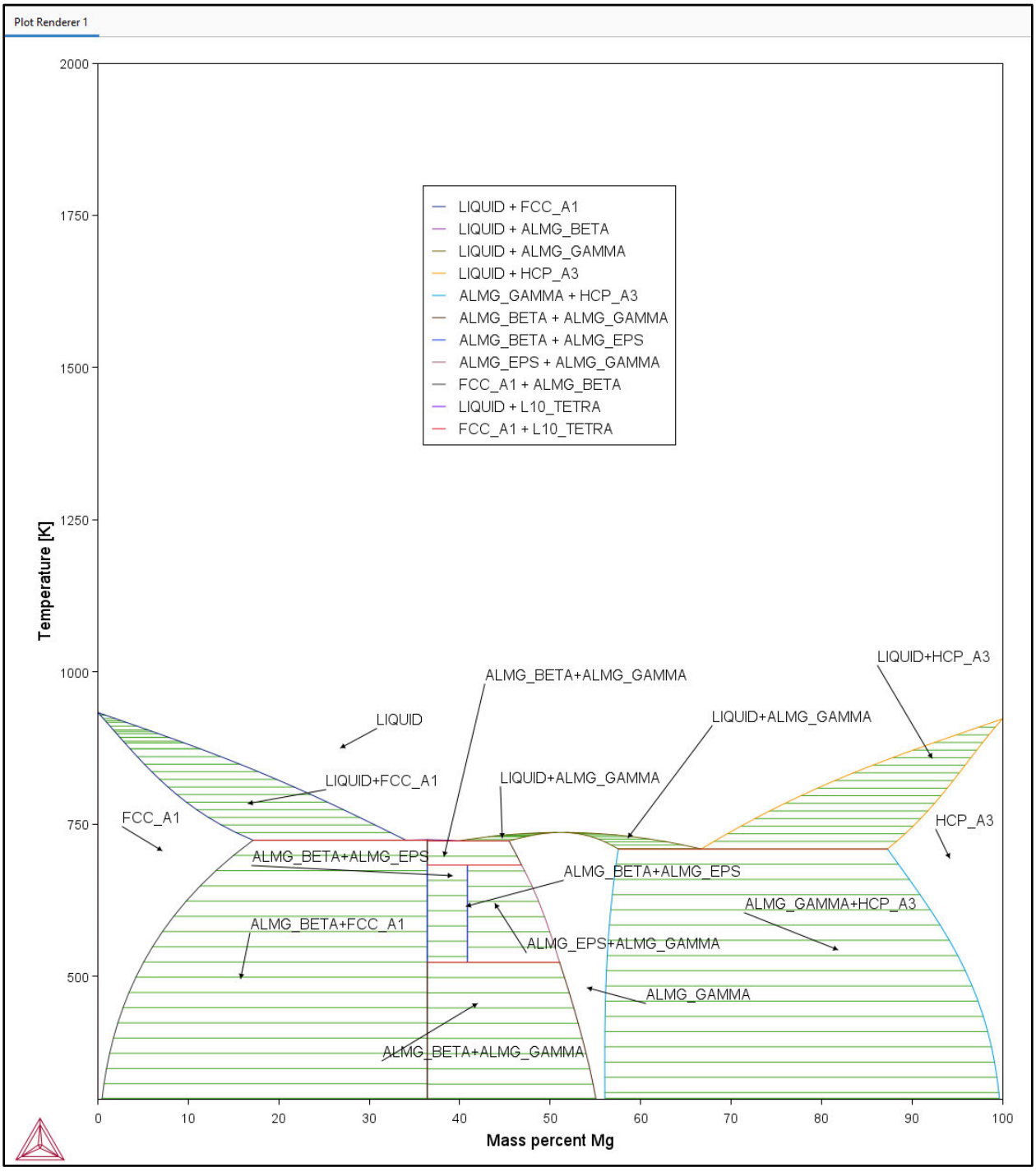


ii) Plot renderer configuration (Setting up the axes, and units and retaining the labels)



(b) **Performing the binary calculation tree and labeling the phases:**



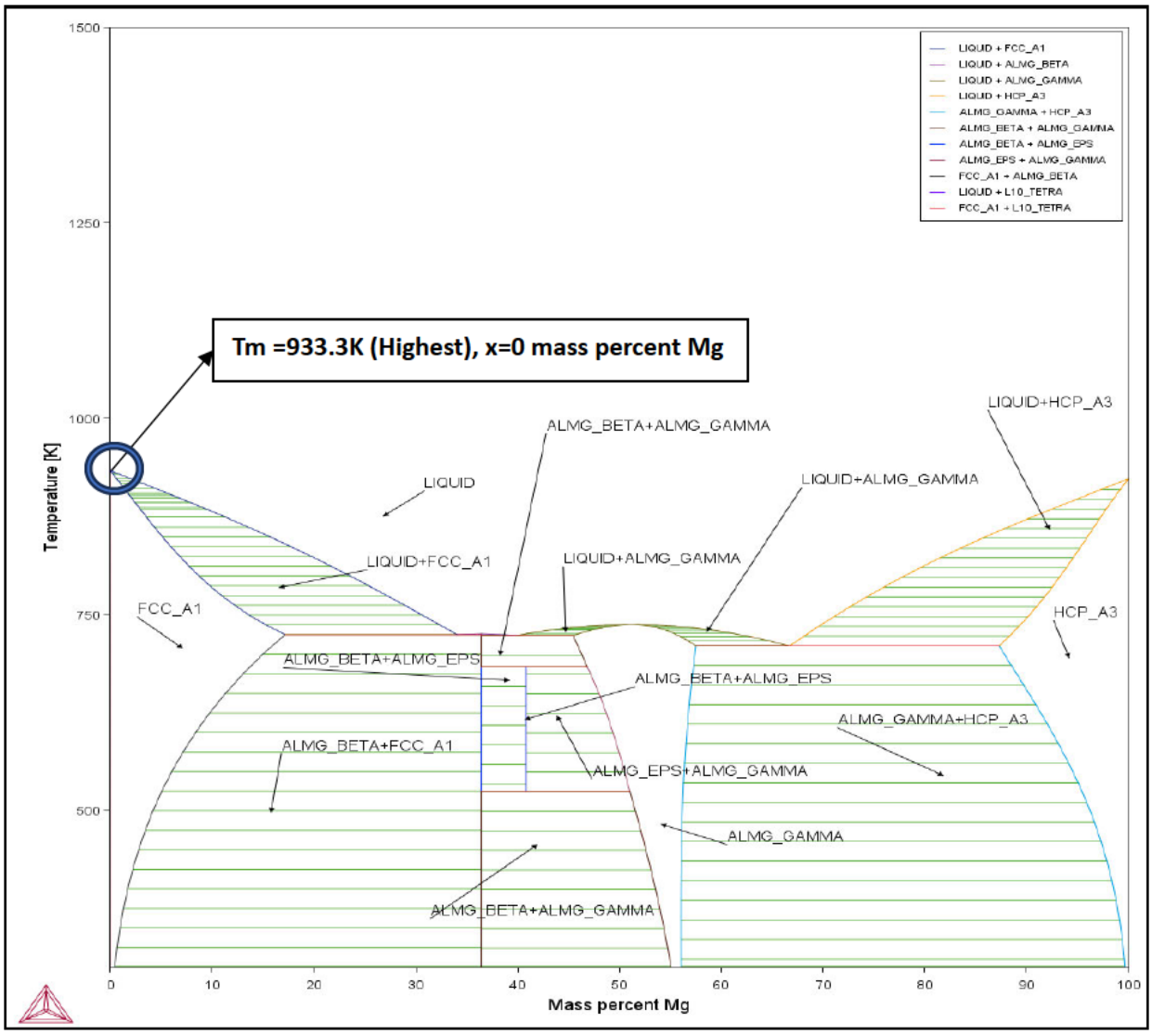


The labels in the above phase diagram were selected by right-clicking on the phase to be labeled and then selecting – "Add label".

The above phase diagram does not go to very high temperatures for the solid phases, so the rest of the calculations will terminate the upper limit of temperature at T= 1500 K.

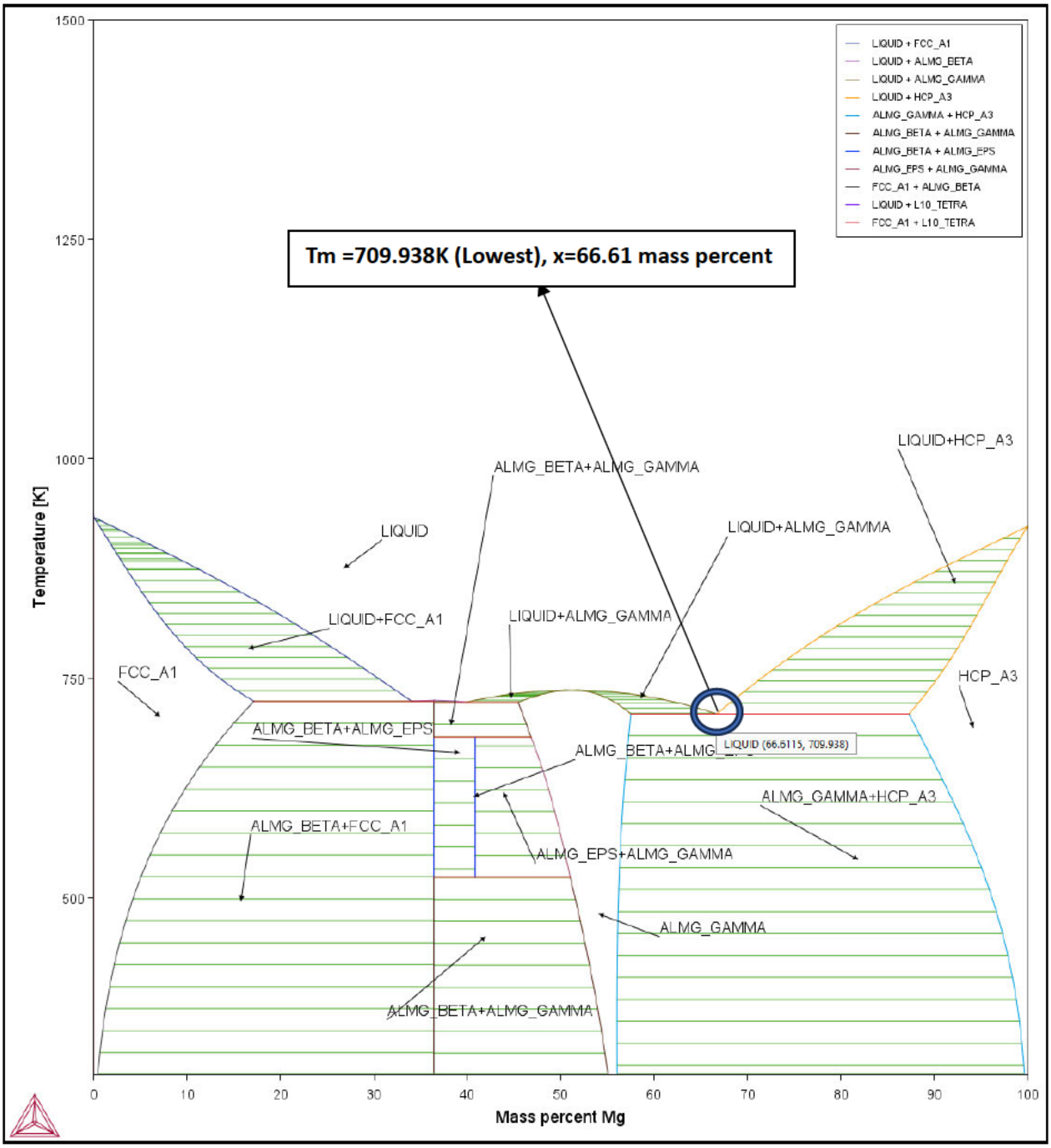
(c) **Highest melting point and corresponding composition:**

The highest melting would correspond to the temperature above which only the liquid phase exists. This corresponds to the pure Al component as seen from the phase diagram. The melting point observed is equal to 933.3 K and agrees with the experimentally reported value in the literature [1]. Corresponding composition= 0 mass percent Mg or 100 mass percent Al.



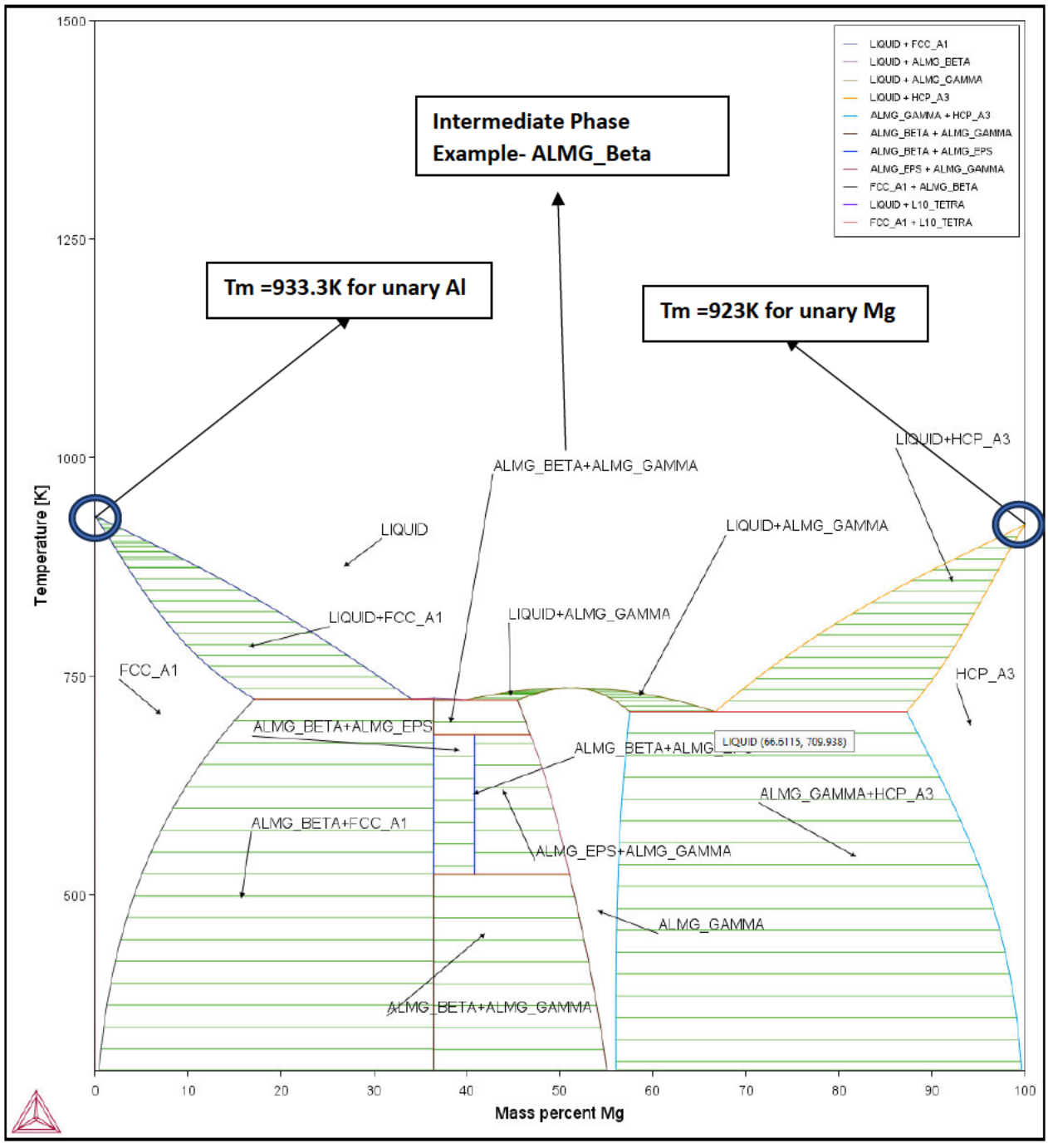
Lowest melting point and corresponding composition:

The lowest melting point corresponds to the temperature below which every possible phase is a solid irrespective of the composition. The lowest melting point for the Al-Mg system is the eutectic point indicated by the arrow in the phase diagram below along with the composition. The values obtained are 709.938K and 66.61 mass percent of Mg, respectively.



Melting point of unary systems:

These are the melting point temperatures corresponding to 0 and 100 mass percent Mg.

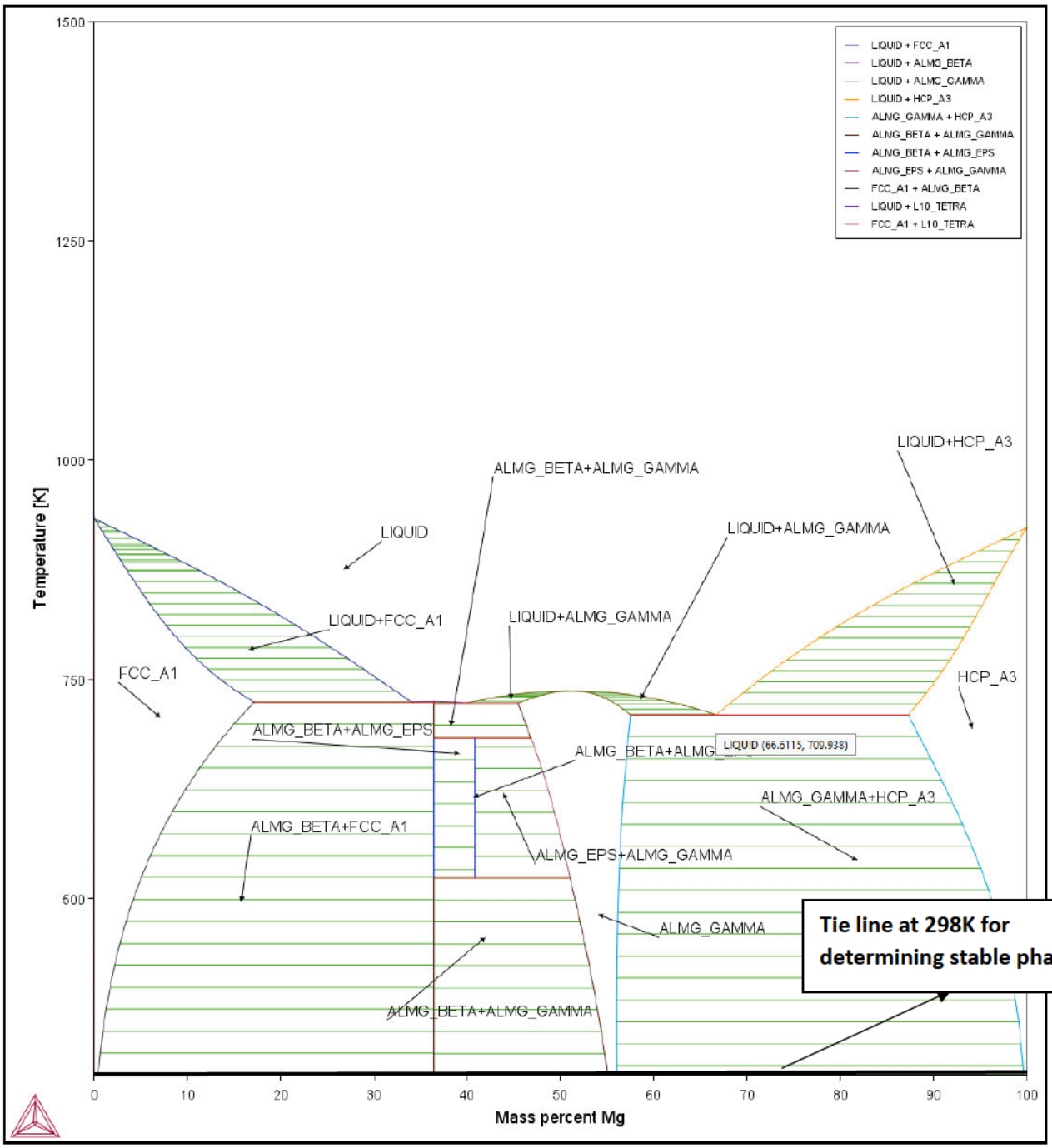


(d) **Intermediate phases in the phase diagram**

The intermediate phases are defined as the ones between the pure components, i.e., the pure Al and pure Mg. These are labeled in the above phase diagram: FCC_A1, ALMG_Beta, ALMG_Gamma, HCP_A3, ALMG_EPS, L_10_Tetra.

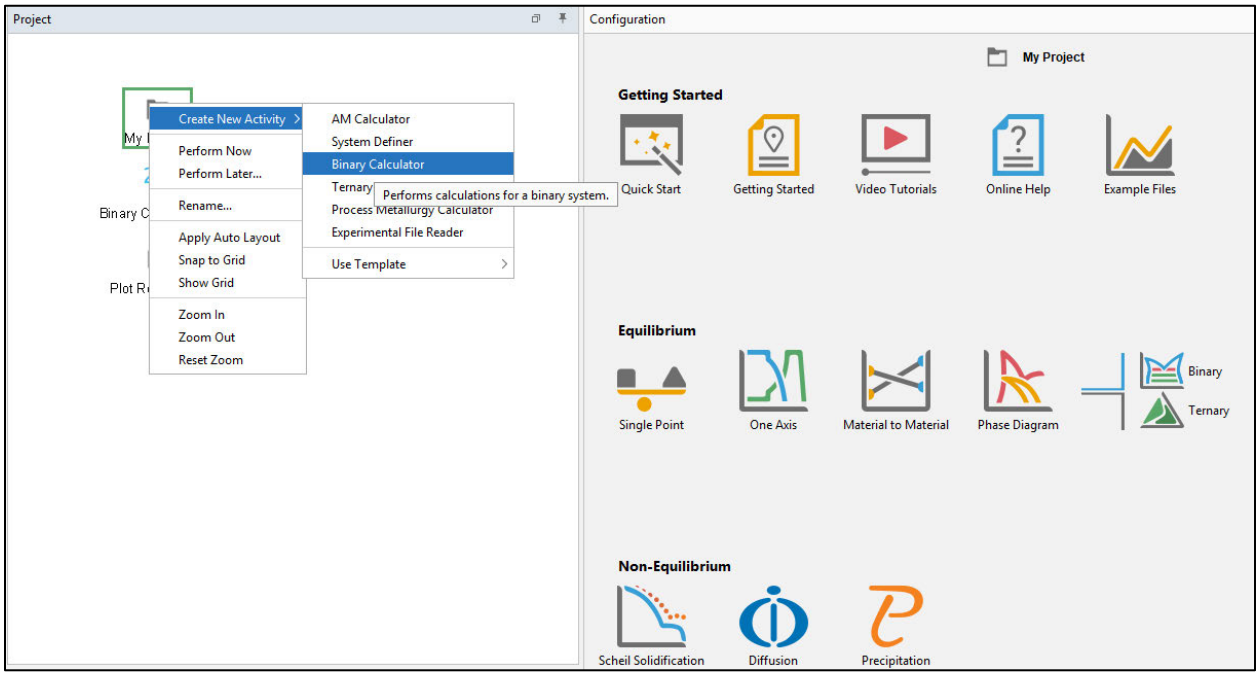
(e) **Stable phases for unary systems at room temperature**

At 298K, the stable phases are FCC_A1, ALMG_Beta, ALMG_Gamma, and HCP_A3.

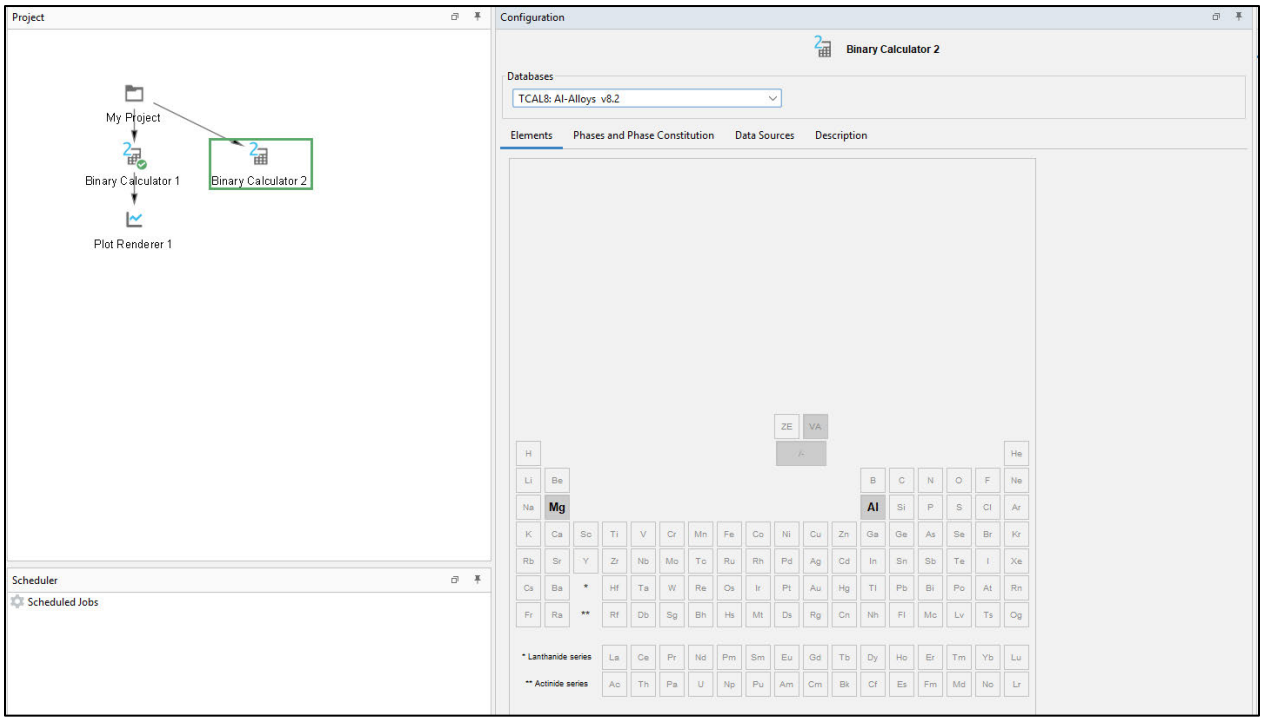


II. Calculation of Gibbs Free Energy

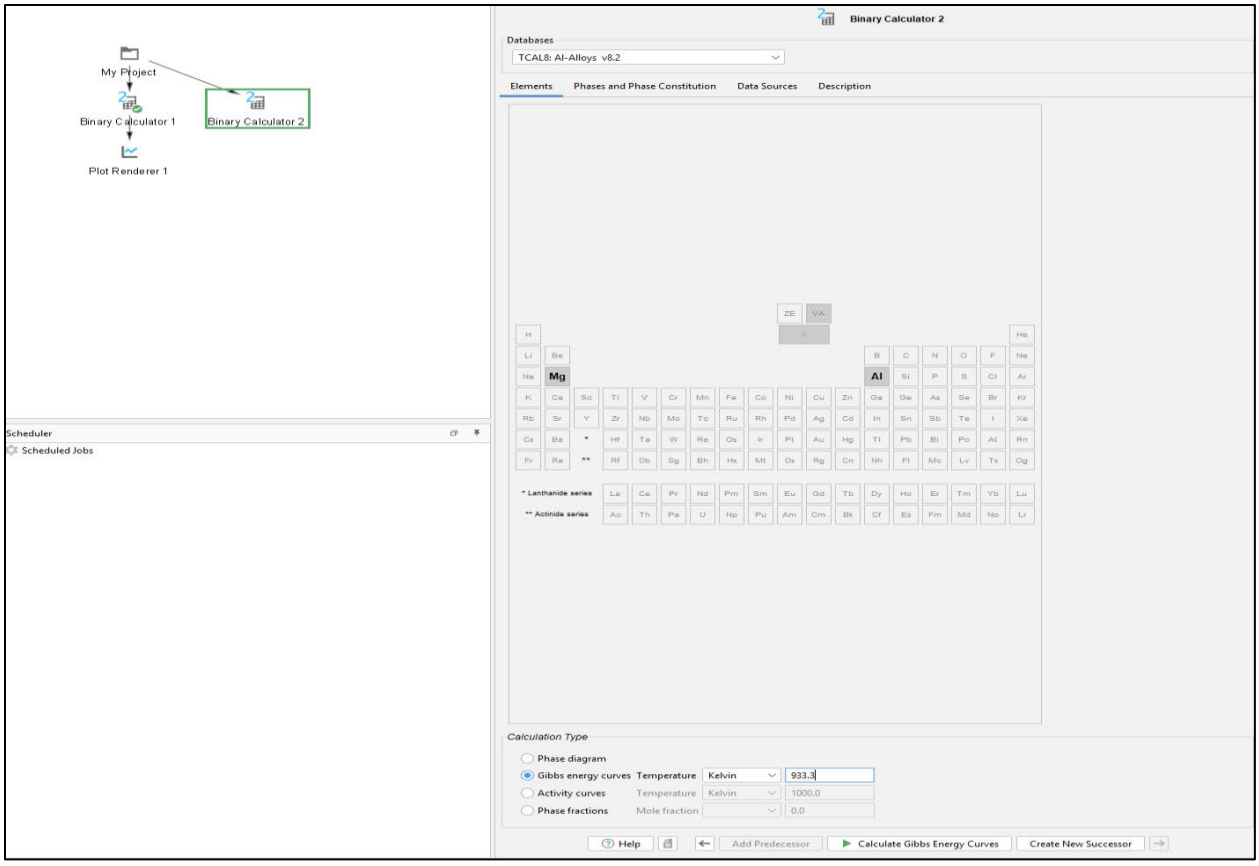
(a) Step 1: Creating a new activity and defining a binary calculator for Gibbs free energy.



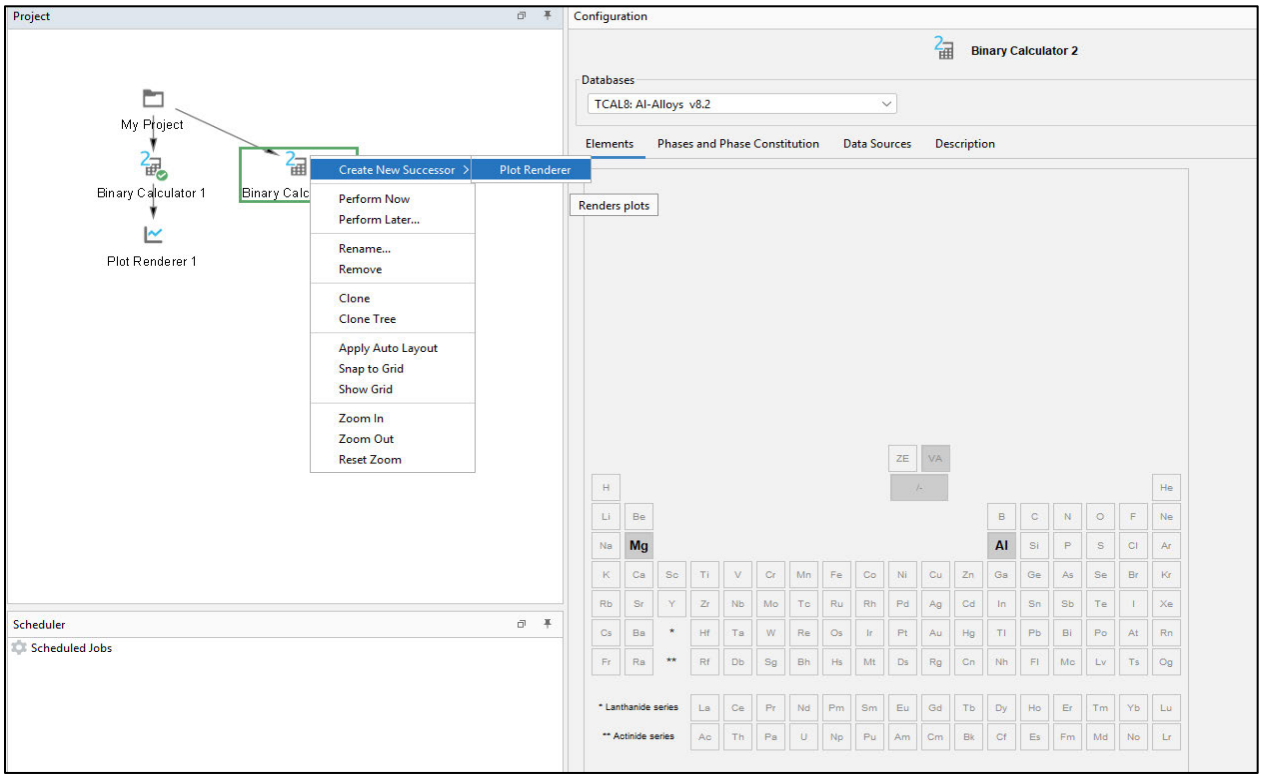
Step 2: Selecting the database and the components for calculation.



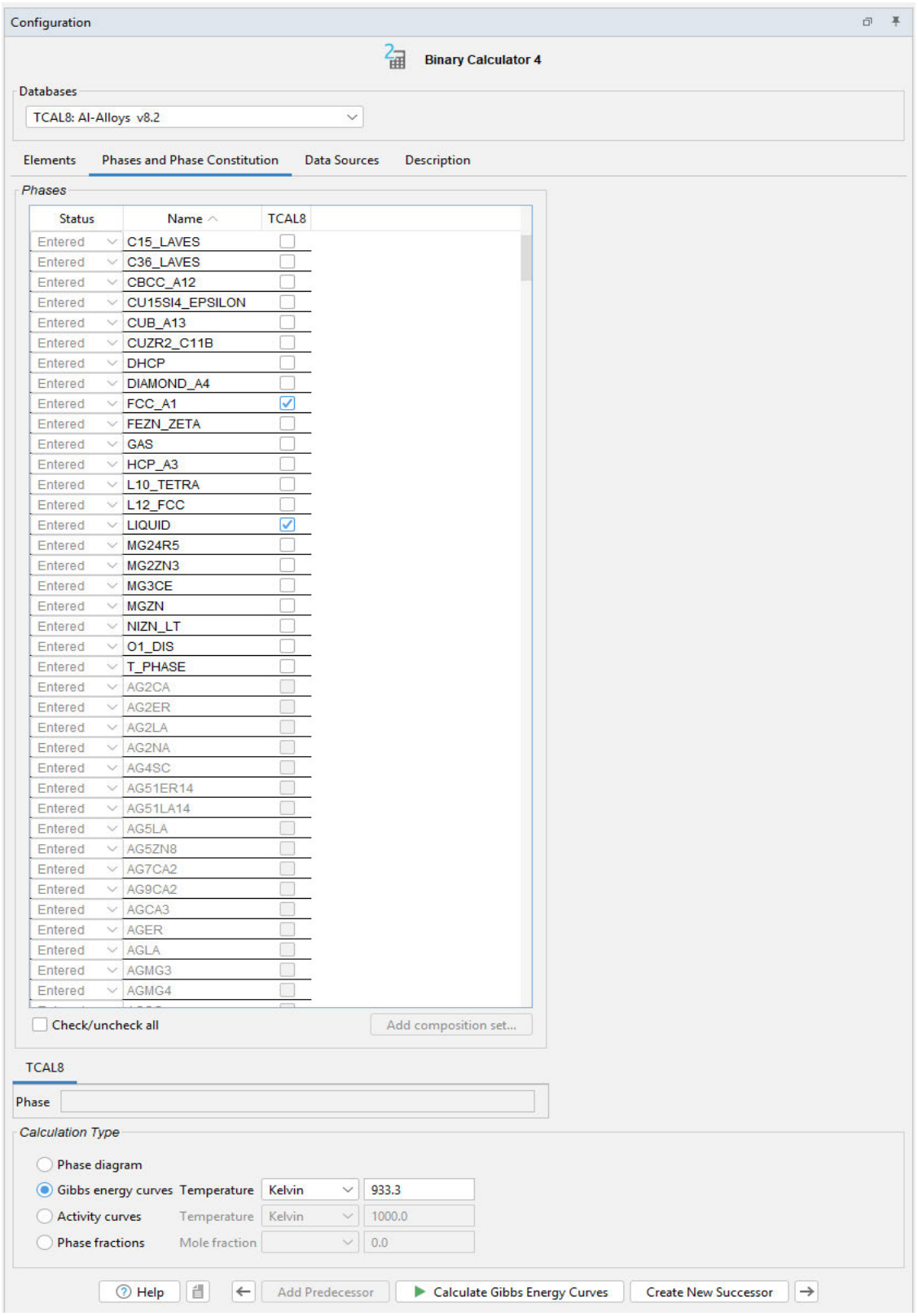
Step 3: Specifying the temperature (Eg., T=933.3K) for the Gibbs free energy curves option in the GUI mode.



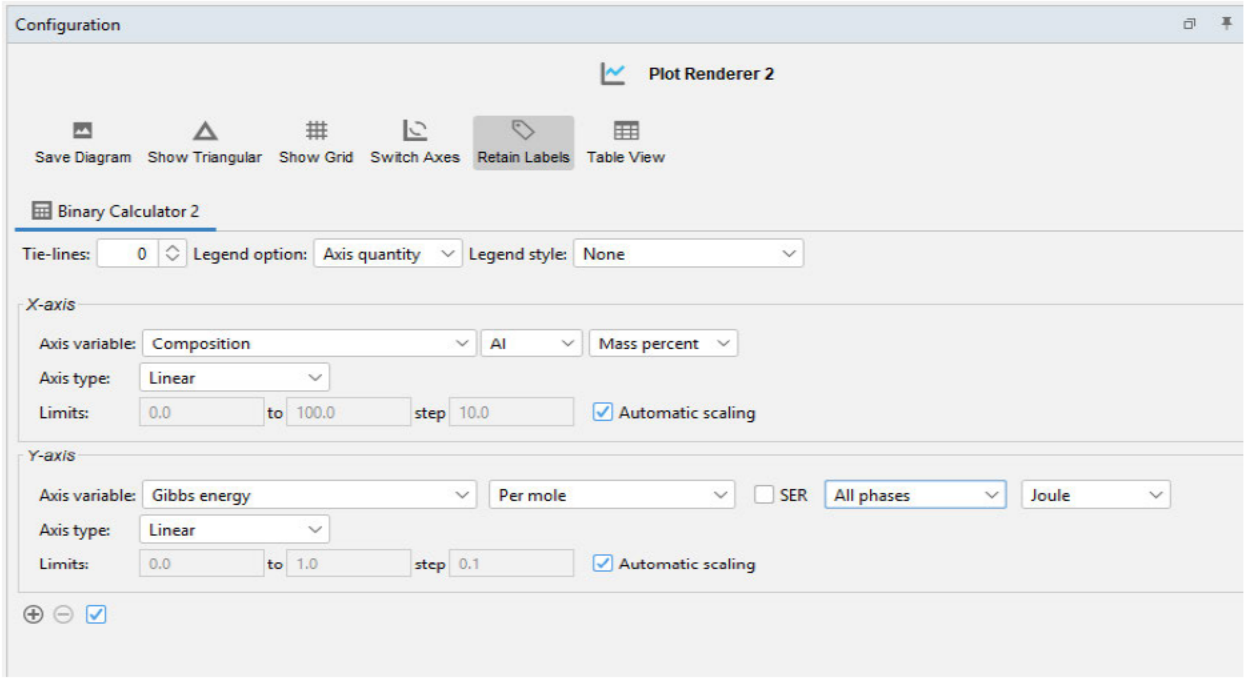
Step 4: Creating a new plot renderer successor for plotting the gibbs energy curves.



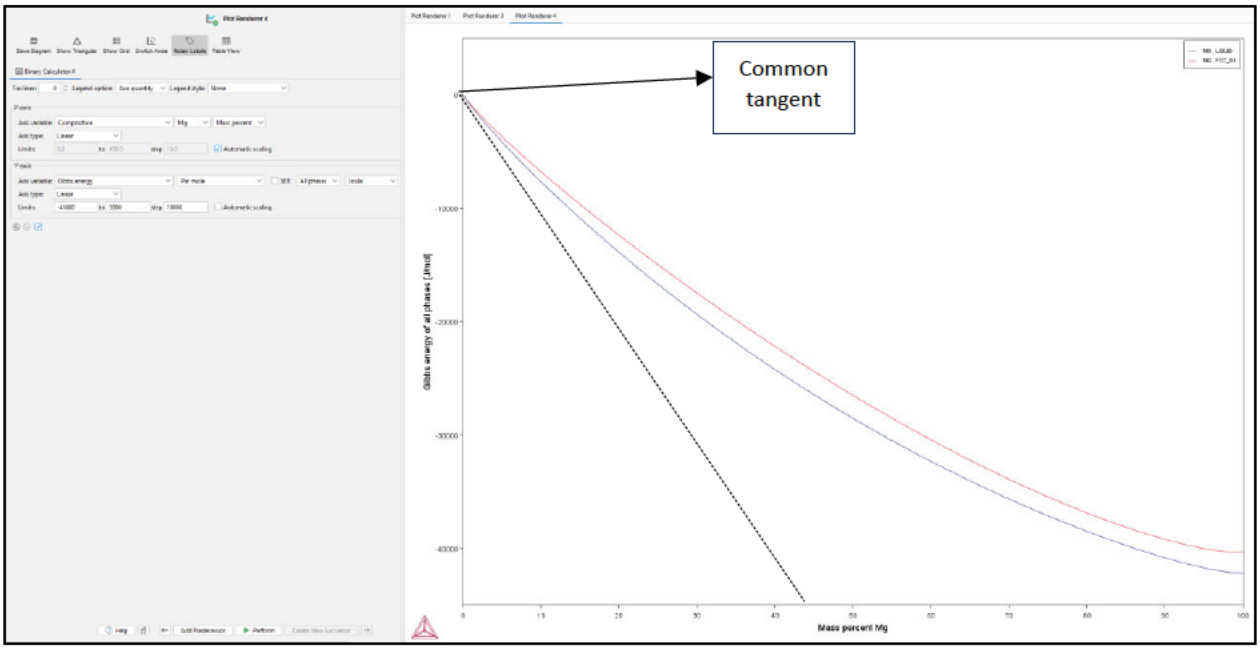
Step 5: We select only two phases that are stable at the highest melting point by looking at the phase diagram.



Step 6: Choosing the appropriate settings in the plot renderer- Axis scaling and units.



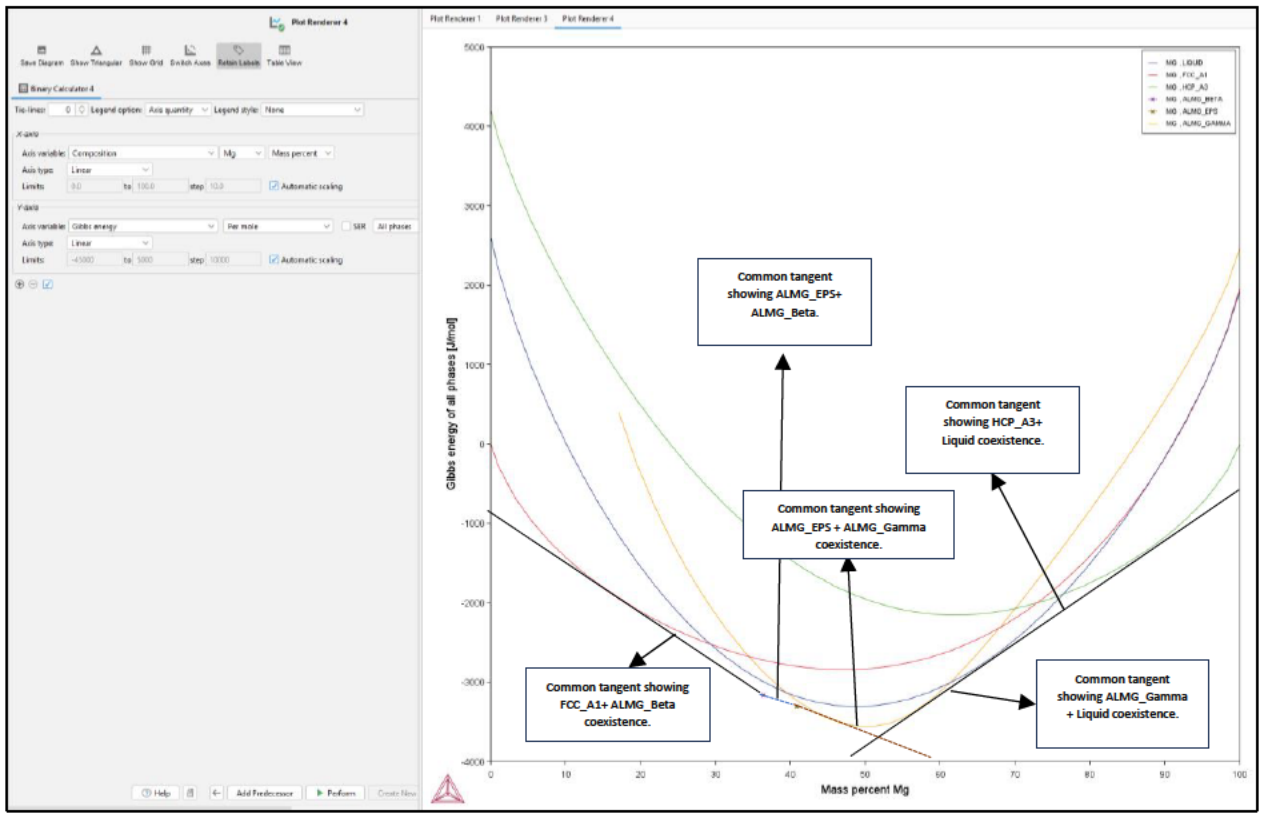
(b) G-X curves at the highest melting point (T_m= 933.3K)



We observe just one common tangent here as we only have the coexistence of liquid in equilibrium with FCC_A1 at the melting point (100% Al).

(c) G-X curves at the lowest melting point (T_m= 709.938K)

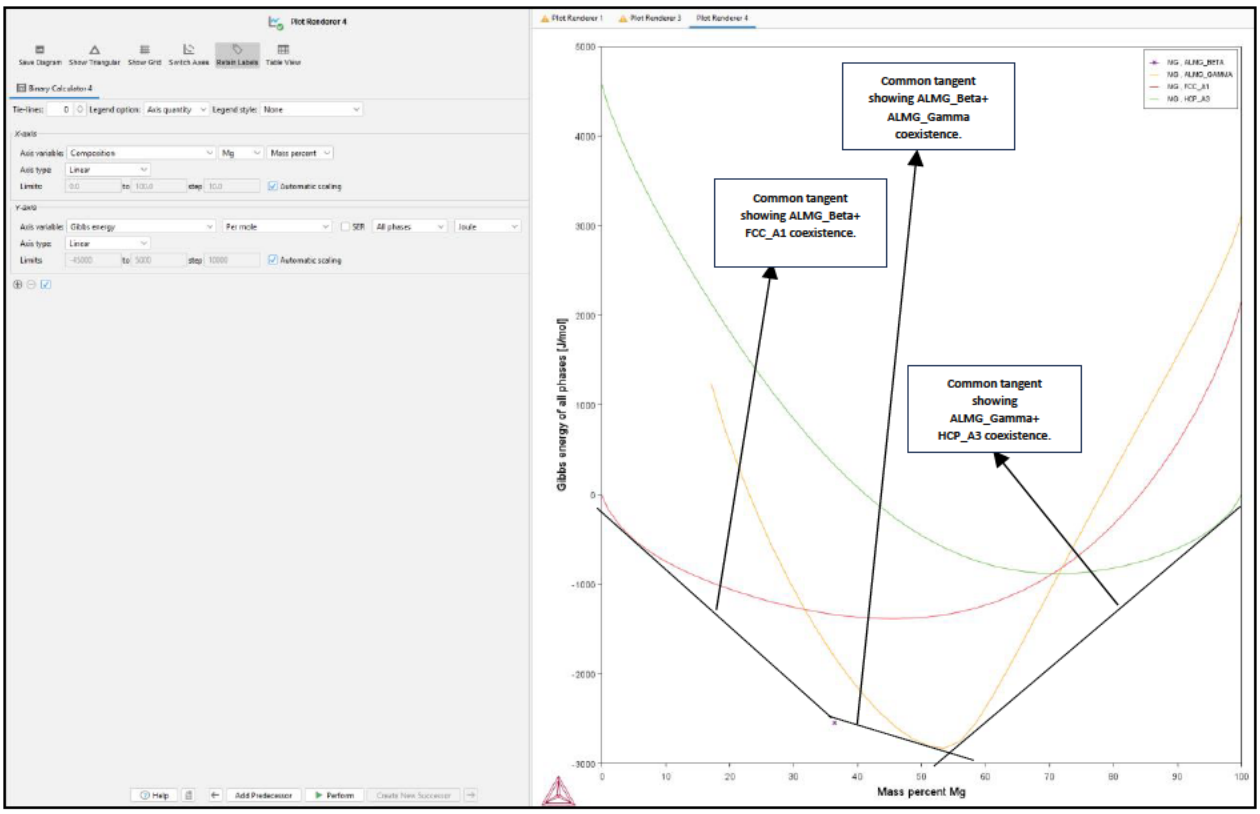
Stable phases/intermediates/compounds at T= 709.938 K according to the phase diagram: FCC_A1, ALMG_Beta, ALMG_EPS, Liquid, ALMG_Gamma, HCP_A3



We observe 5 common tangents showing the coexistence of different phases. The lowest Gibbs free energy curves and the common tangents between the curves can be connected to obtain the **convex hull**.

(d) G-X curves at 200K above room temperature (T= 498K)

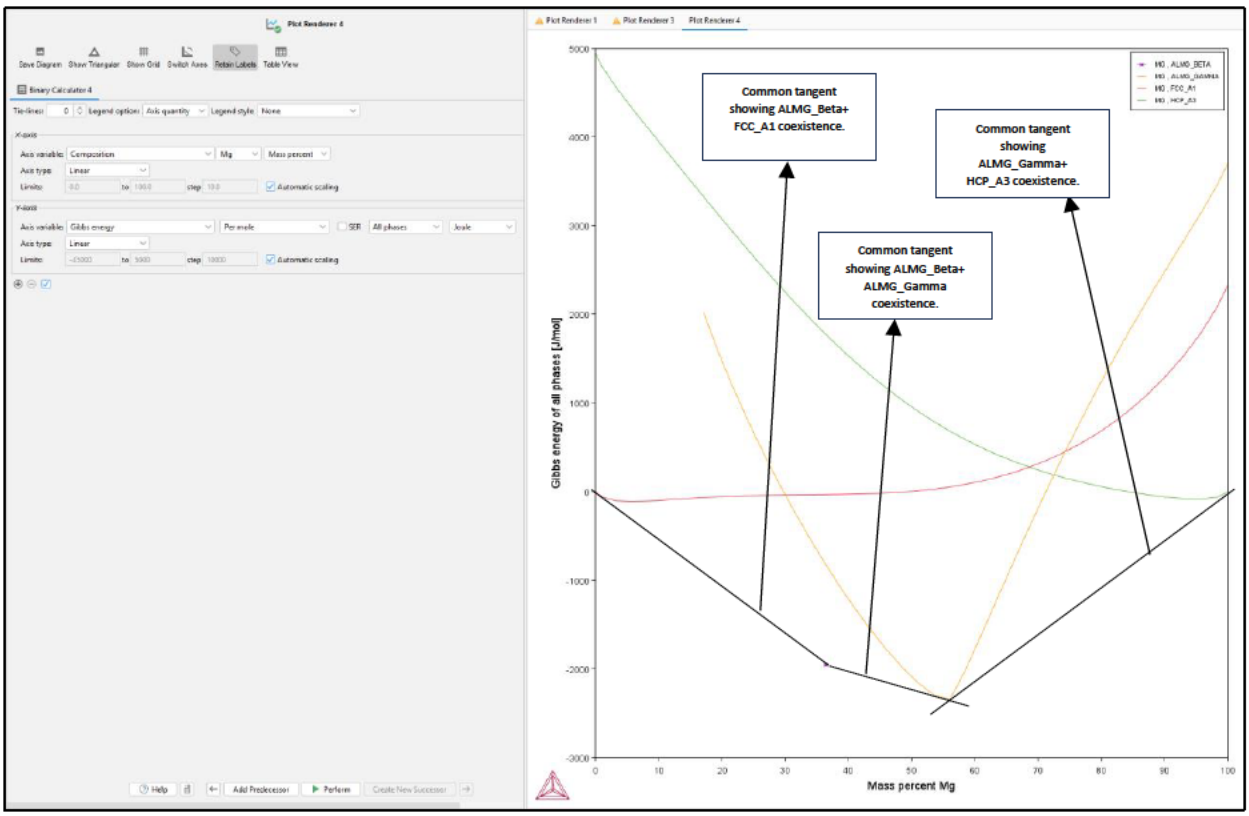
Stable phases/intermediates/compounds at T= 498K according to the phase diagram: FCC_A1, ALMG_Beta, ALMG_Gamma, HCP_A3



We observe 3 common tangents showing the coexistence of ALMG_Gamma+ HCP_A3, ALMG_Beta+ FCC_A1, and ALMG_Beta + ALMG_Gamma. The * point is for the compound ALMG_Beta which has the lowest energy in the left region of the GX curve. The convex hull can again be obtained by connecting the lowest Gibbs energy curves and the common tangents from curve to curve.

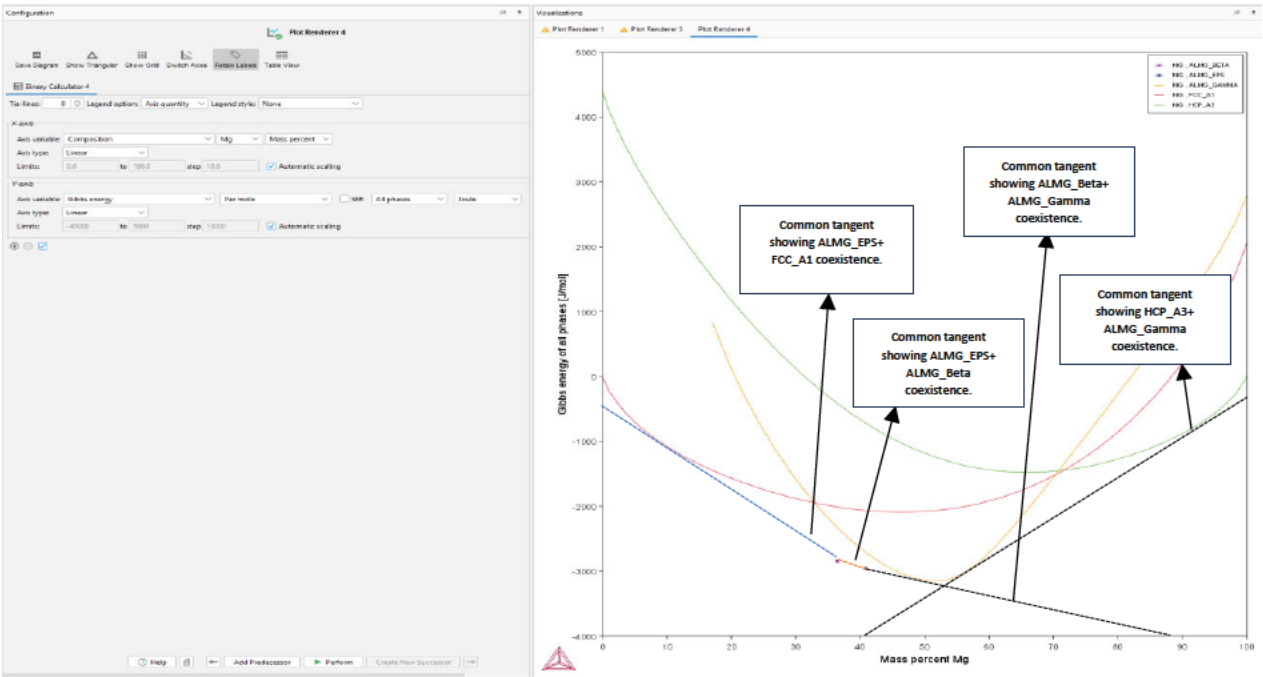
(e) G-X curves at room temperature (T= 298K)

Stable phases/intermediates/compounds at T= 498K according to the phase diagram: FCC_A1, ALMG_Beta, ALMG_Gamma, HCP_A3



We observe 3 common tangents showing the coexistence of ALMG_Gamma+ HCP_A3, ALMG_Beta+ FCC_A1, and ALMG_Beta + ALMG_Gamma.

(f) G-X curves at room temperature (T= 600K)



III. Calculation of the Activity

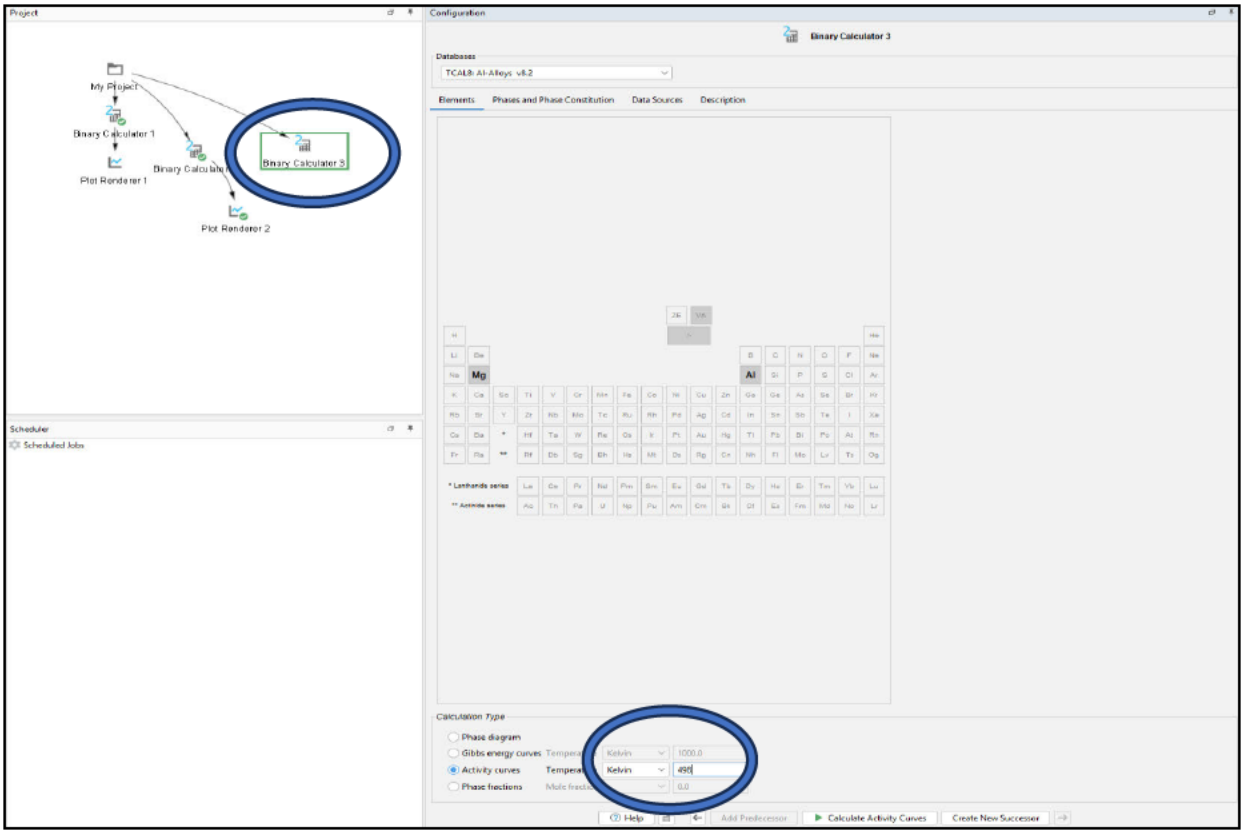
(a) At T=498 K, the stable phases according to the phase diagram are as follows: FCC_A1, ALMG_Gamma, and HCP_A3.

ALMG_Beta: It is a vertical line in the phase diagram indicating a compound, so the activity calculation is erroneous during the calculation using Thermocalc.

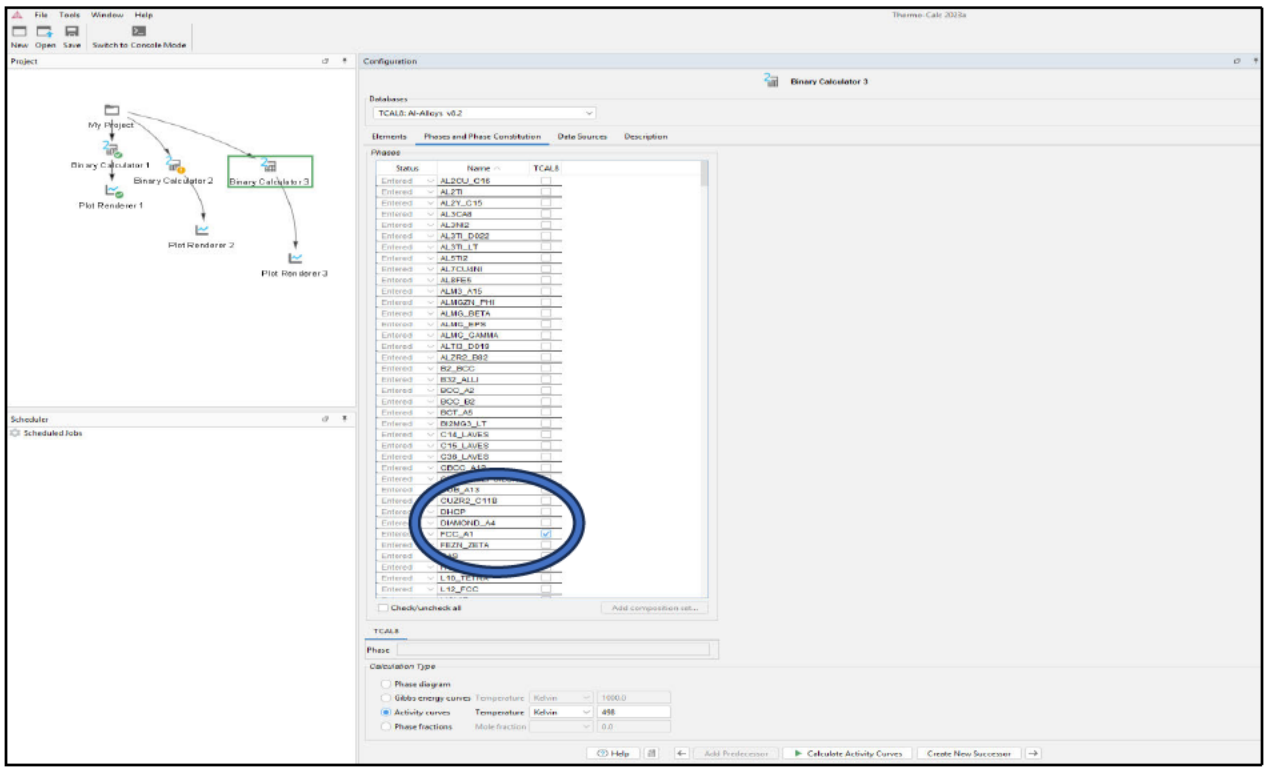
- **Activity of Al in FCC_A1**

Steps to calculate the activity curves using the binary calculator in Thermocalc:

Step 1: Creating a new binary calculator for activity calculation and selecting the relevant temperature (Eg., 498K).

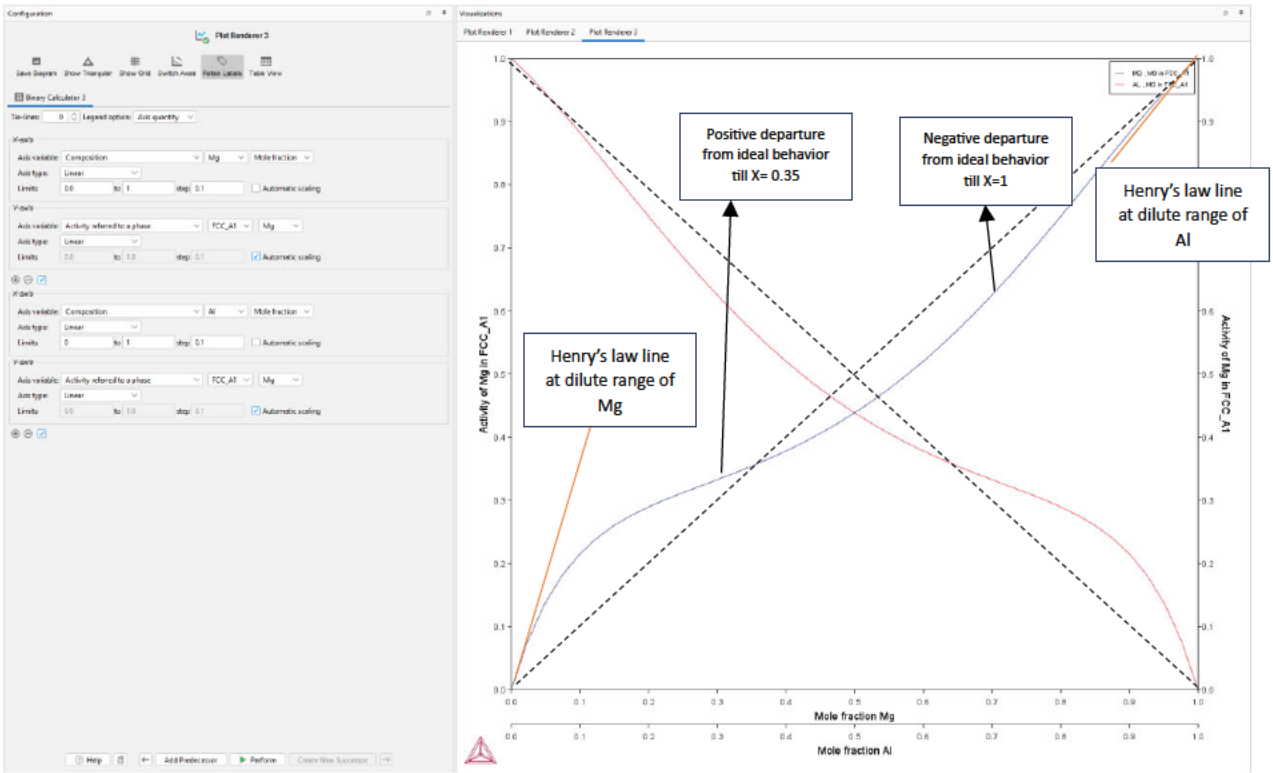


Step 2: Selecting the stable phases at the relevant temperature that were previously determined by drawing a tie line to the phase diagram at that temperature.

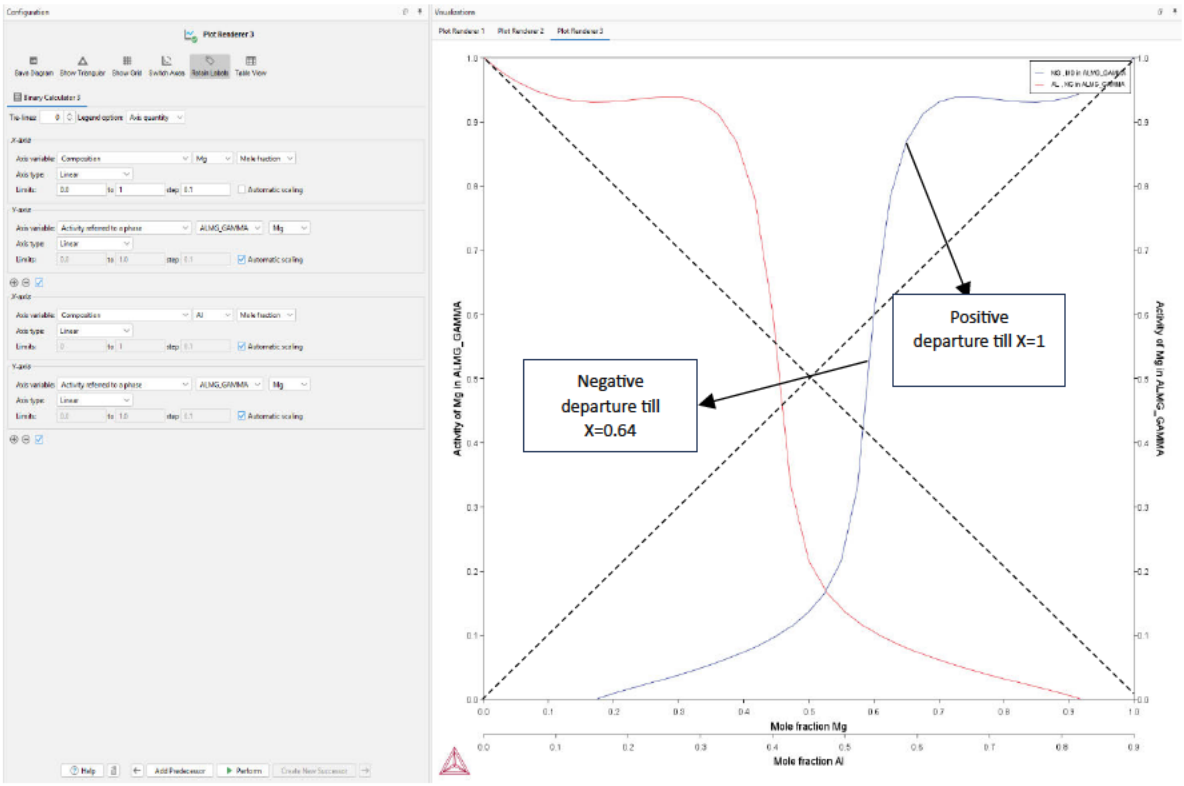


Step 3: Plotting the aX curve of the components in the stable phases

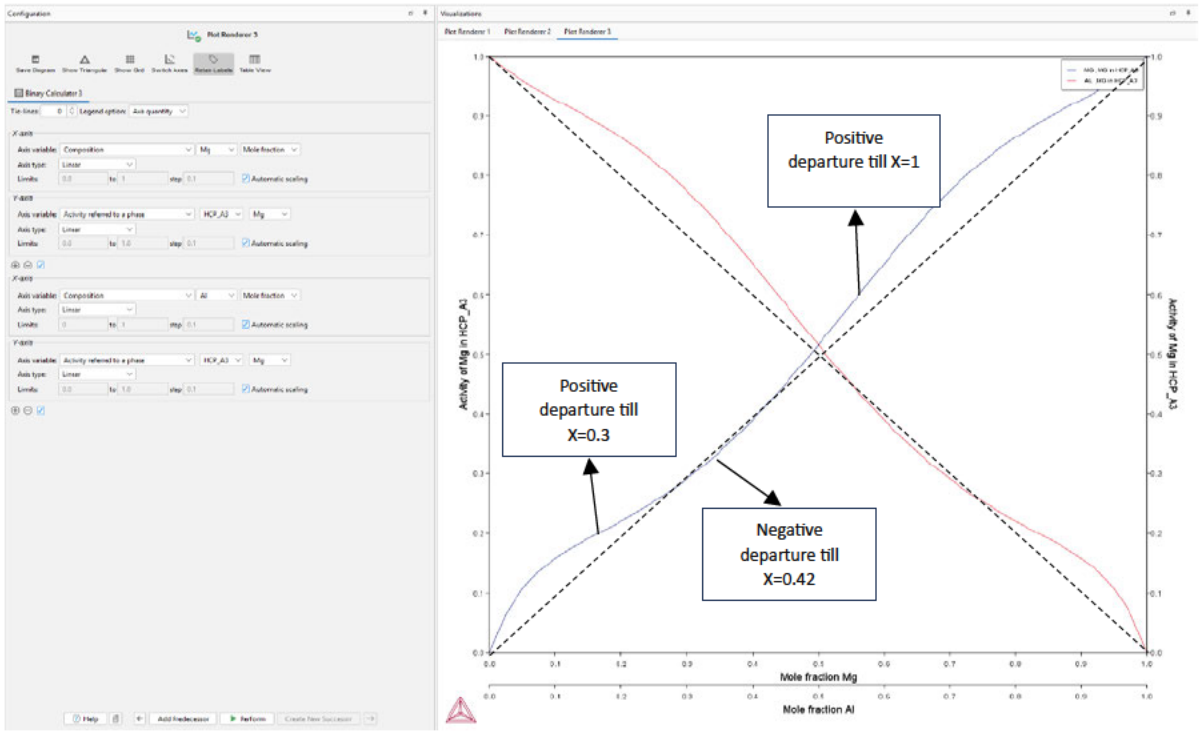
Mg in FCC_A1:



Mg in ALMG_Gamma:

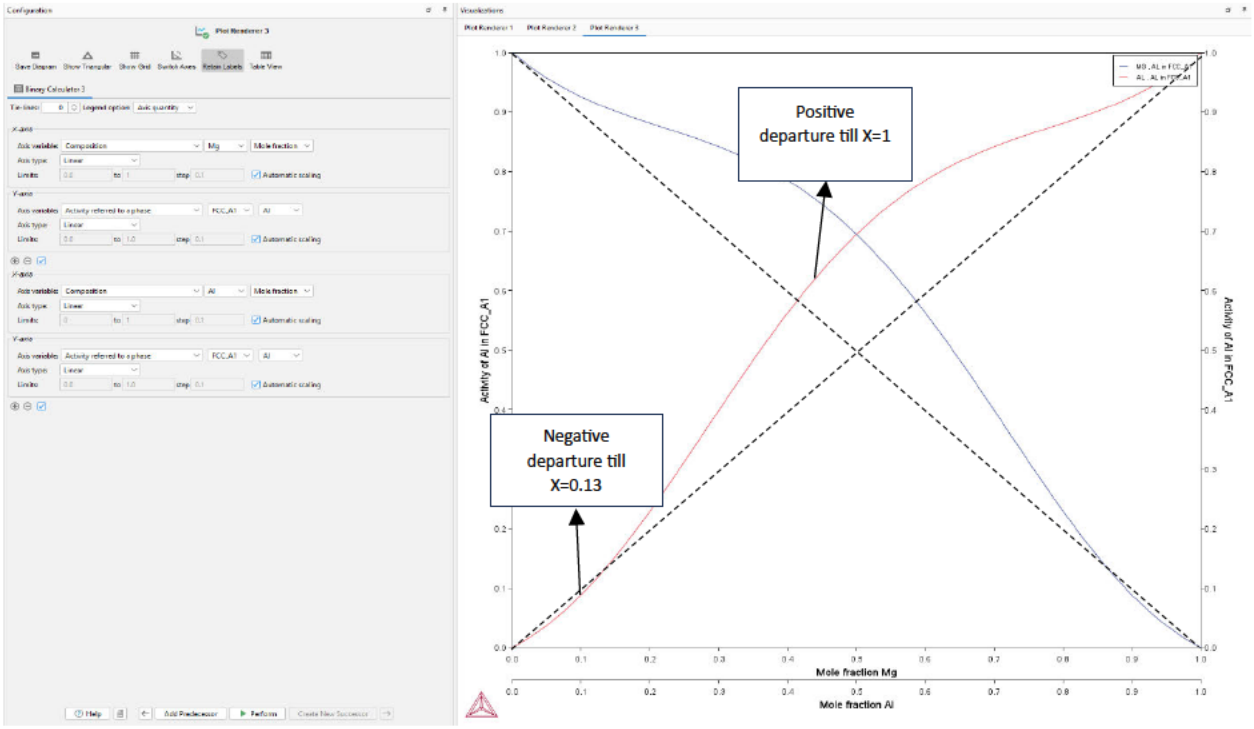


Mg in HCP_A3:

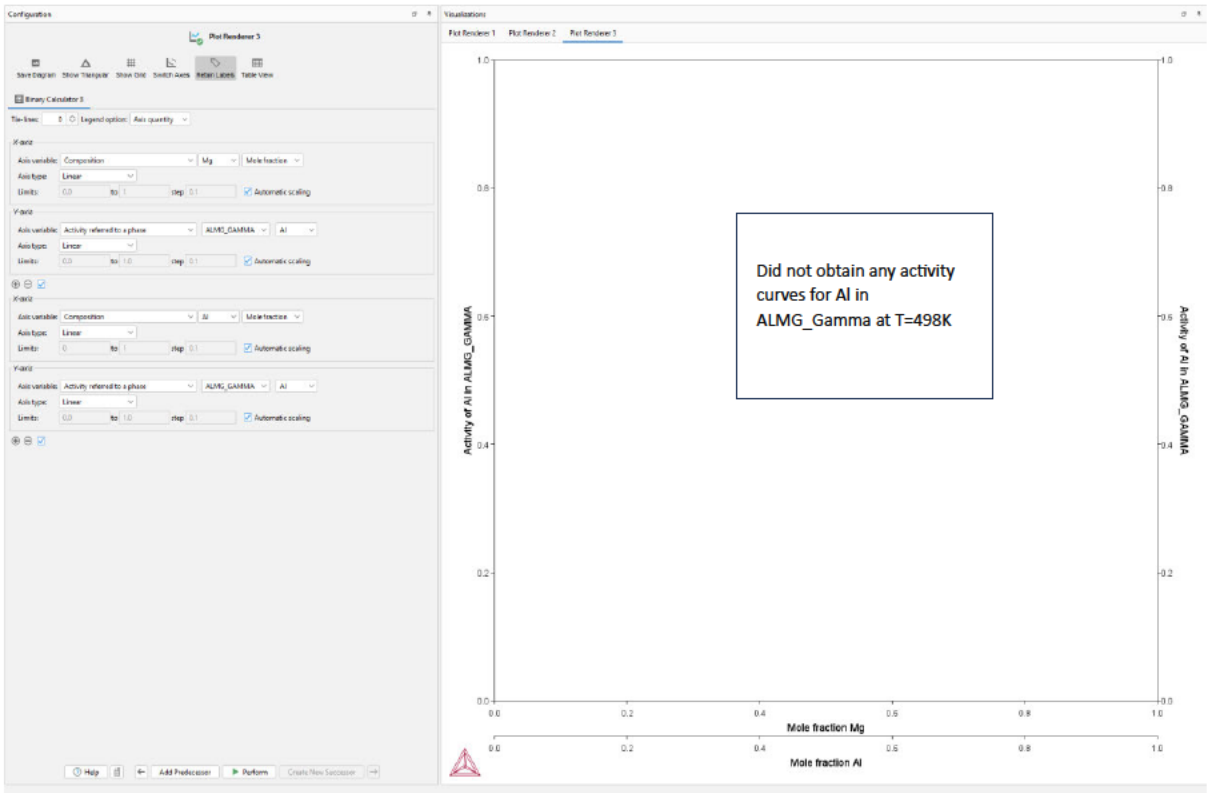


Step 4: Plotting the aX curve of Al in the stable phases

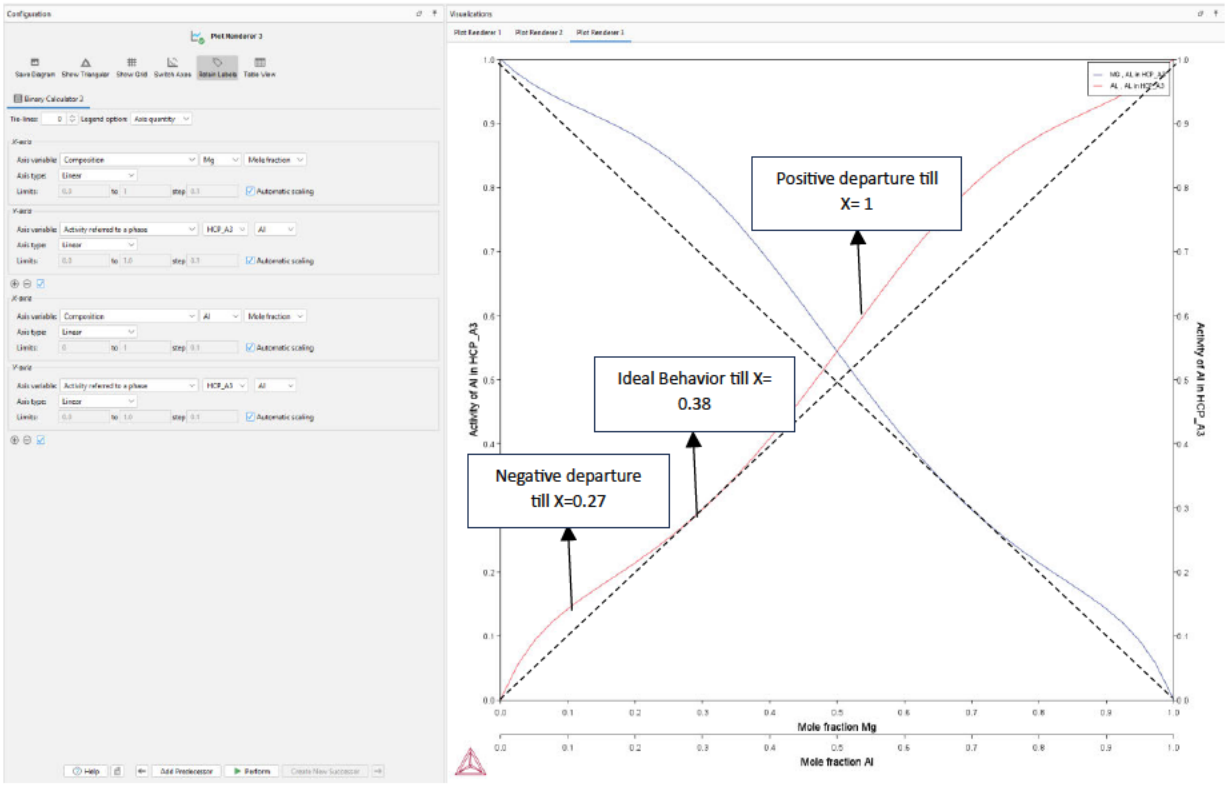
Al in FCC_A1:



Al in ALMG_Gamma:



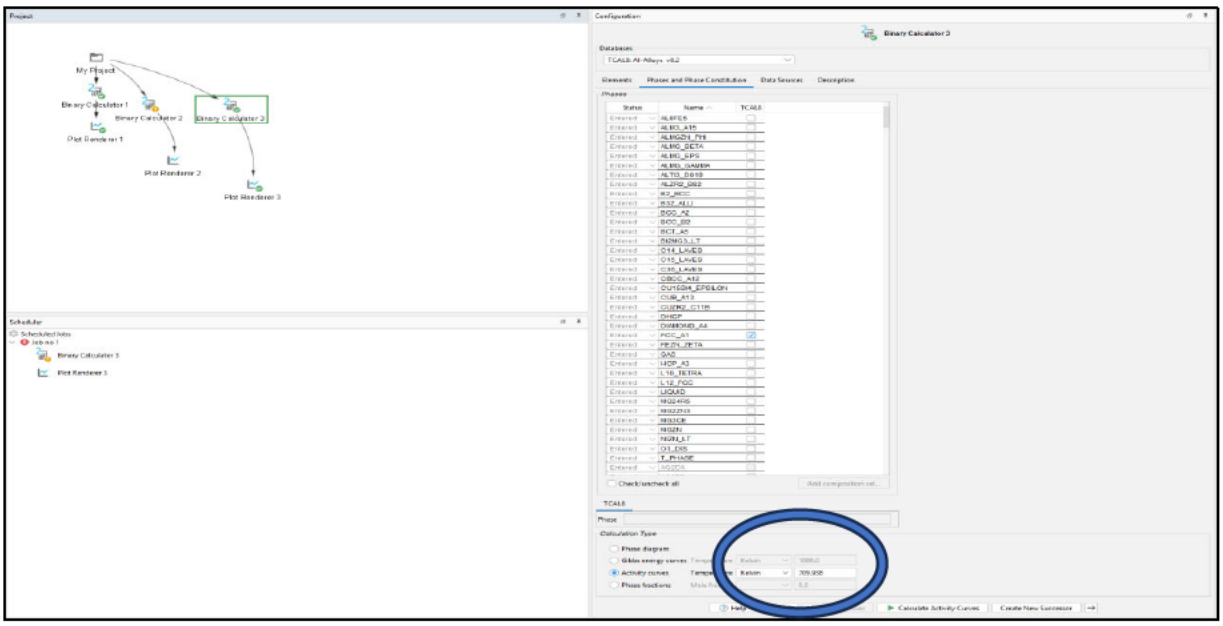
Al in HCP_A3:



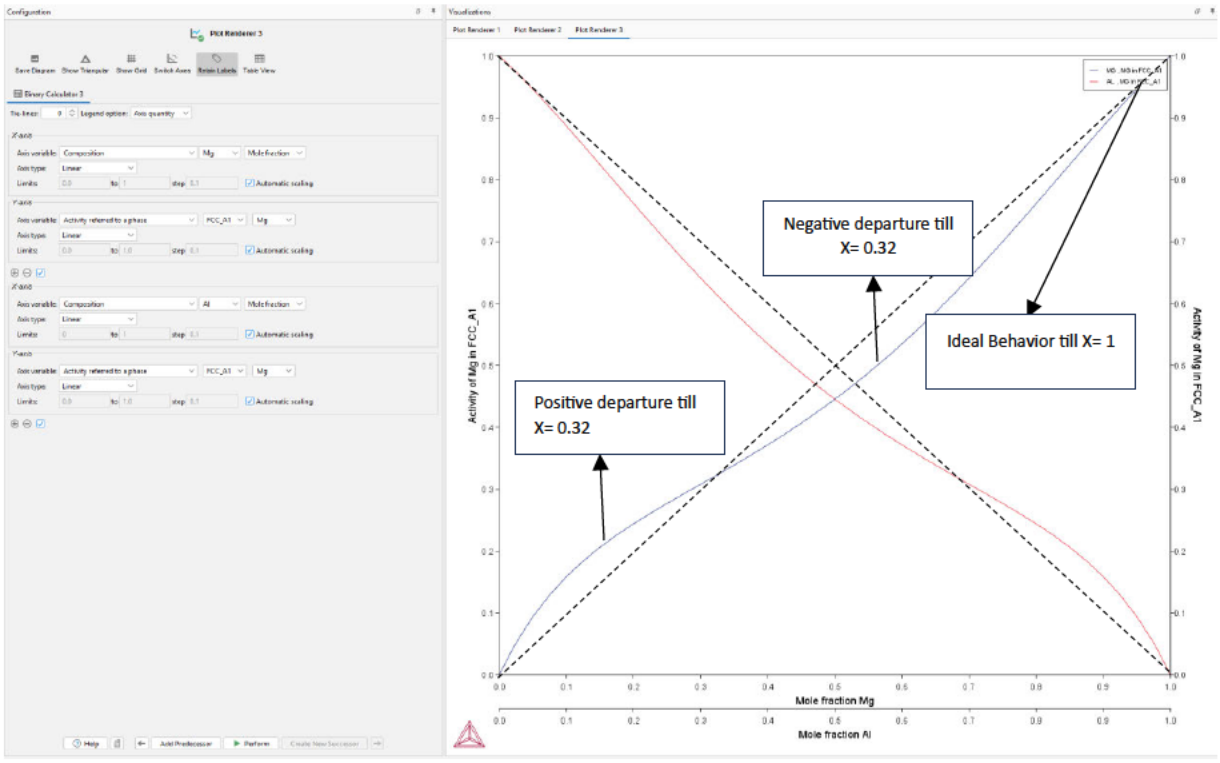
(b) At T=709.938 K, the stable phases according to the phase diagram are as follows: FCC_A1, Liquid, ALMG_Gamma, and HCP_A3.

The ALMG_Beta and ALMG_EPS are vertical lines indicative of compounds.

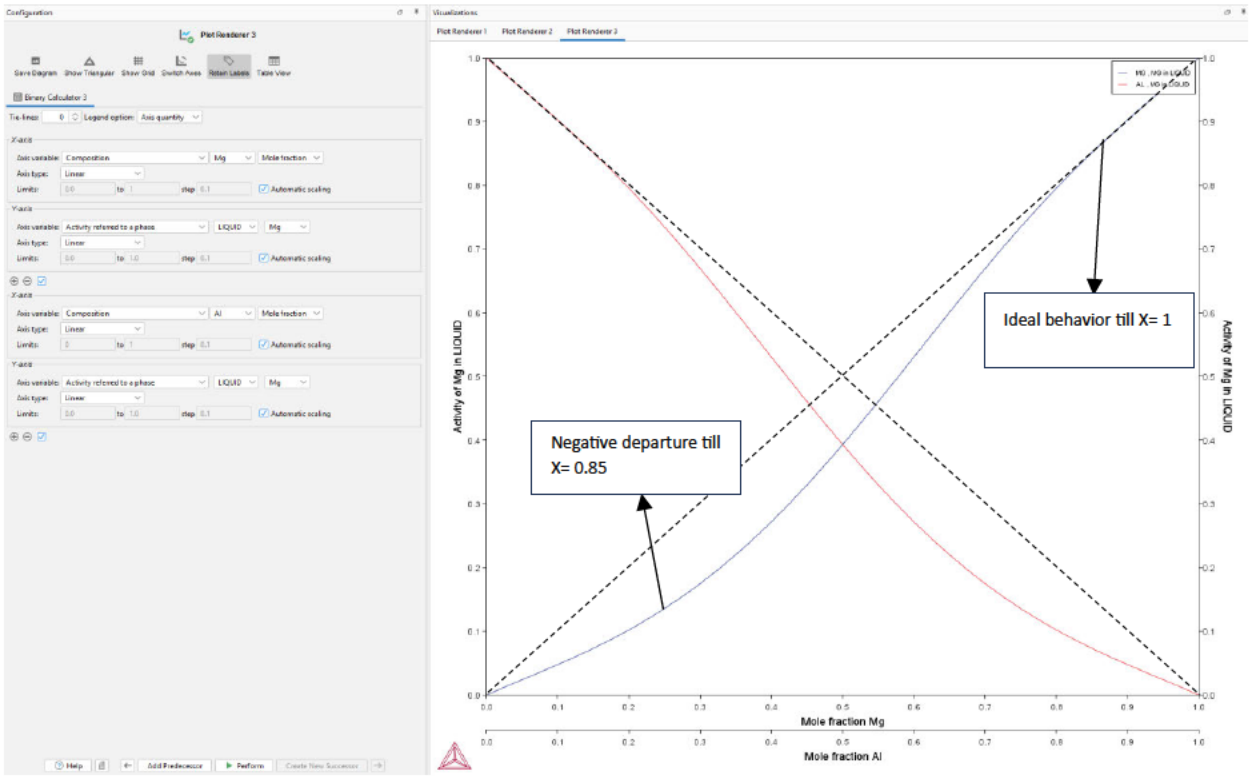
Calculation Step (Selecting lowest melting point temperature):



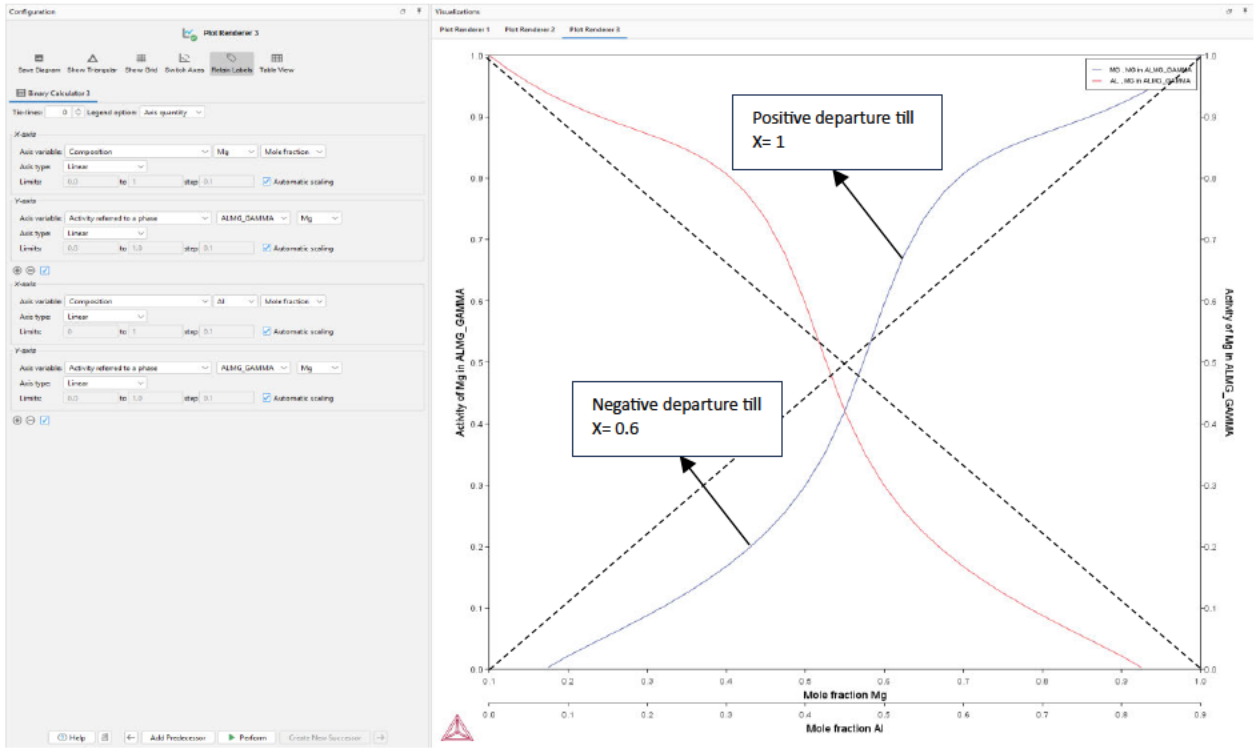
Mg in FCC_A1:


Negative departure till
X= 0.32
Ideal Behavior till X= 1
Positive departure till
X= 0.32
Activity of Mg in FCC_A1
Mole fraction Mg
Mole fraction Al

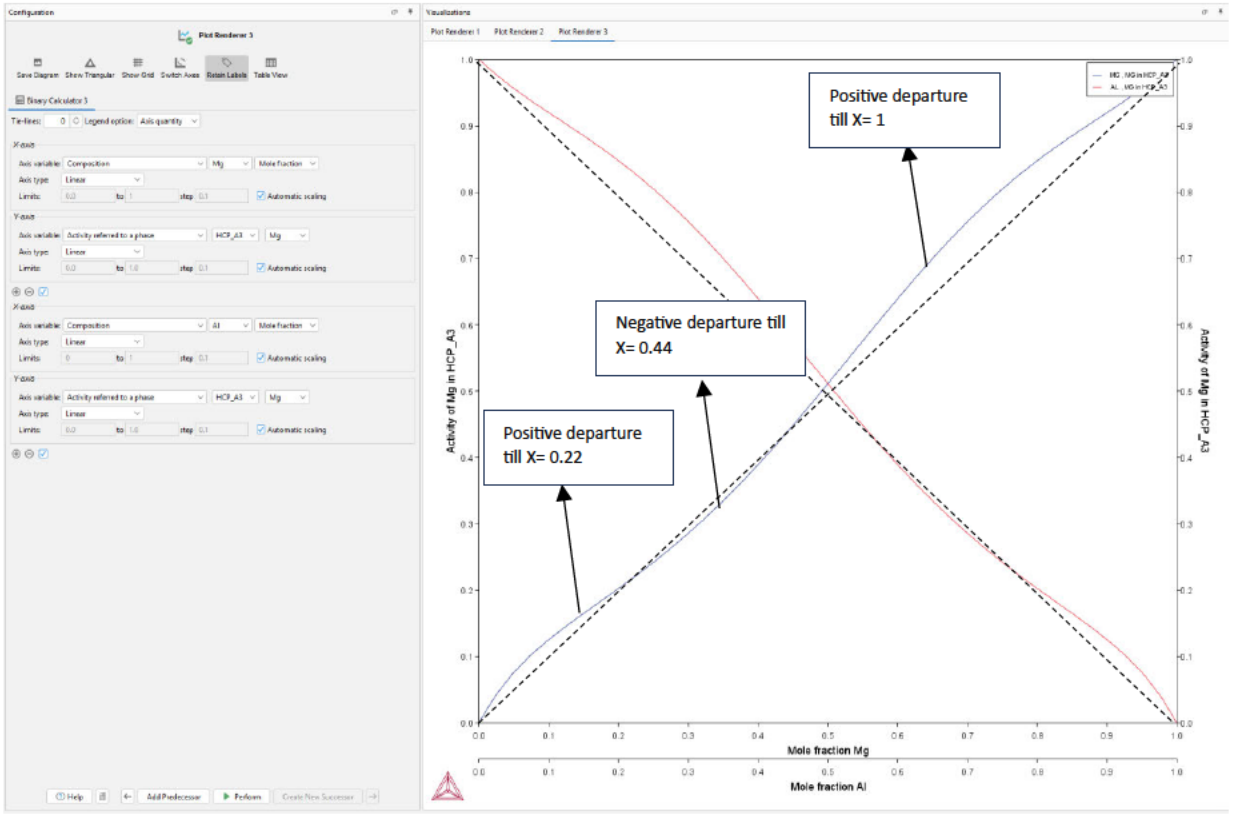
Mg in Liquid:



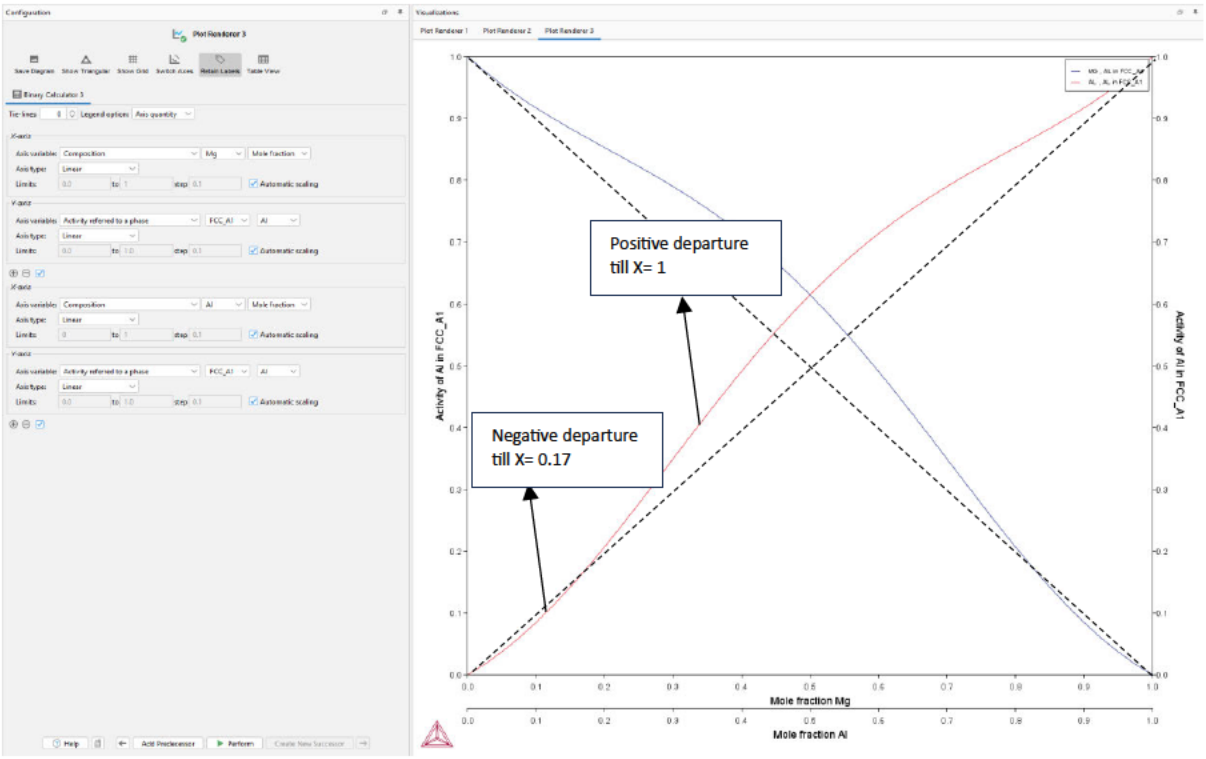
Mg in ALMG_Gamma:



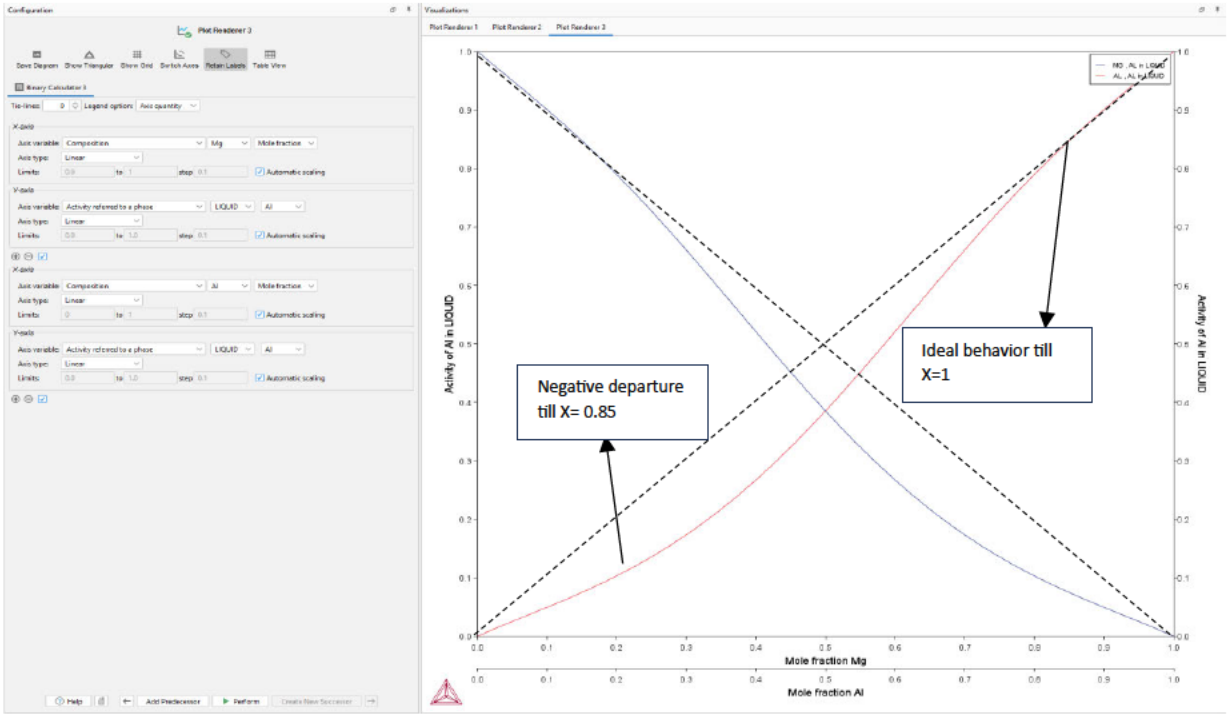
Mg in HCP_A3:



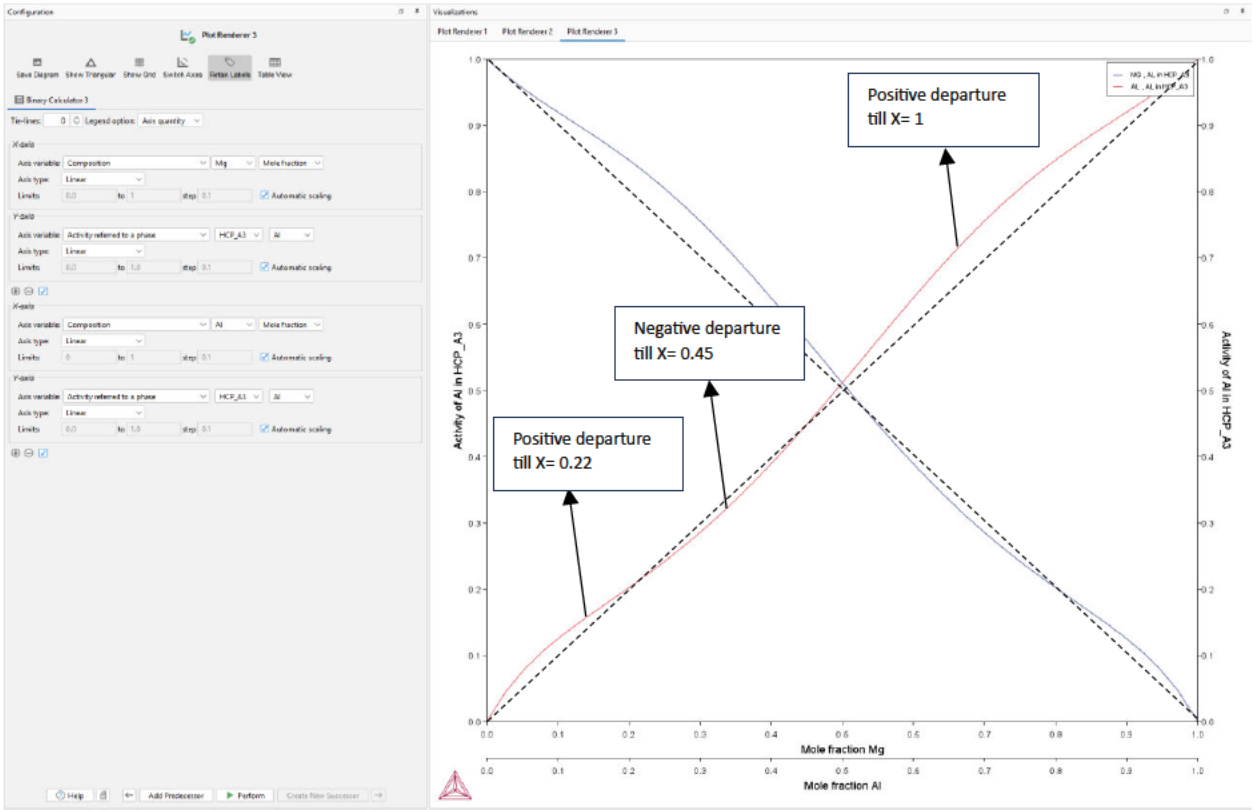
Al in FCC_A1:



Al in Liquid:



Al in HCP_A3:



References:

1. ***Thyssenkrupp Materials Website:*** ***https://www.thyssenkrupp-materials.co.uk/melting-point-of-aluminium***