

CME-572: HW5/Final Project Report



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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	<ol style="list-style-type: none">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

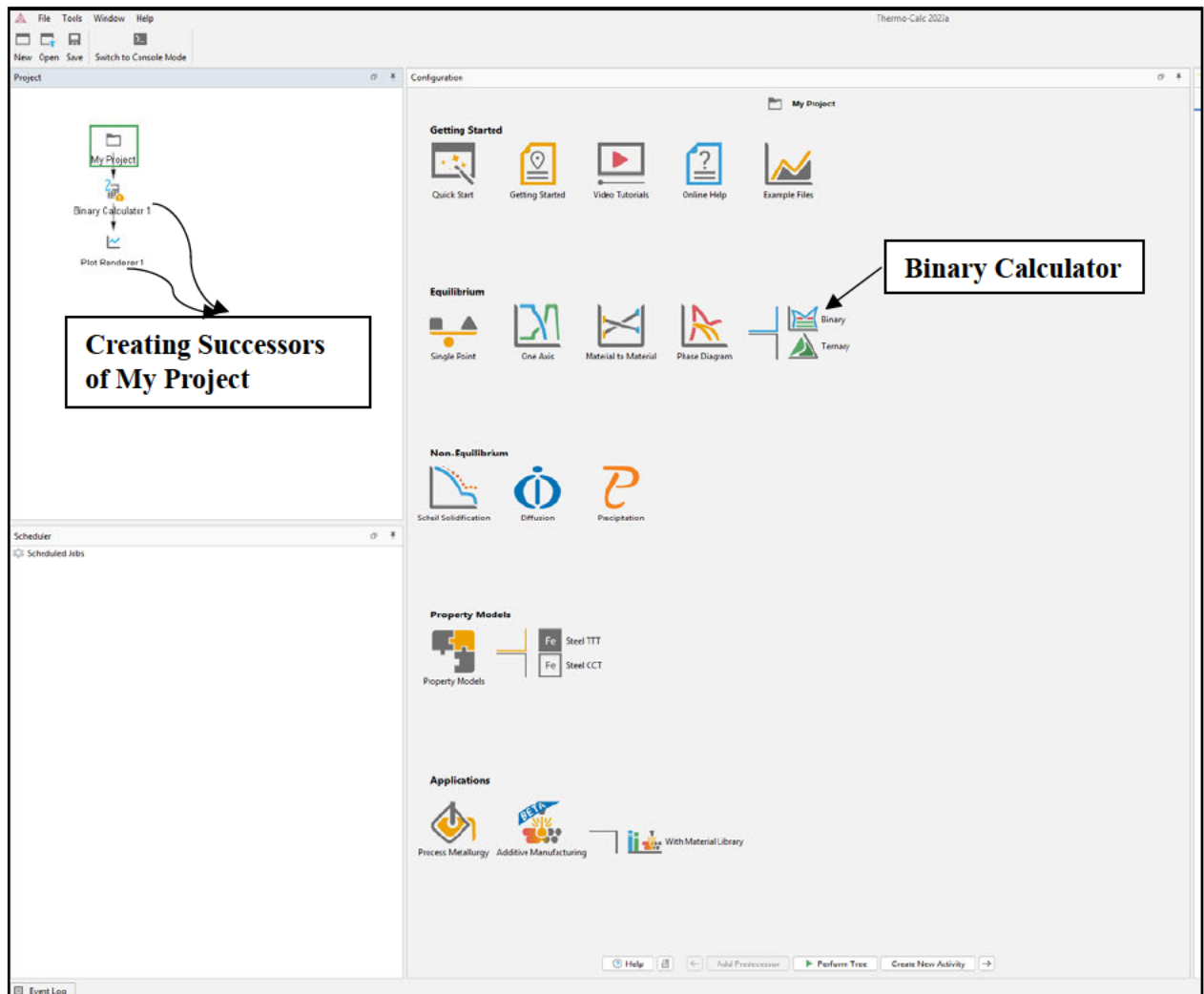
I. Calculation of the Phase Diagram

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 screenshot displays the 'Elements' tab of the TCAL8 software. A text box at the top center reads 'Defining the system by choosing the elements'. Two arrows point from this box to the 'Mg' and 'Al' elements in the periodic table. The periodic table includes standard elements, as well as the Lanthanide series (La to Lu) and Actinide series (Ac to Lr). The 'Mg' element is highlighted in the second row, eighth column, and the 'Al' element is highlighted in the third row, thirteenth column.

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.

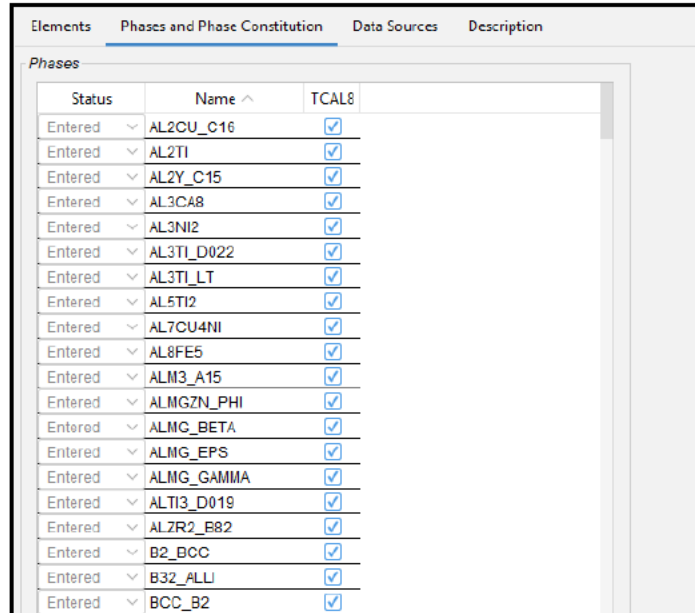
For the binary calculation, the maximum allowable elements are two which can be selected in any order.

3. Setting up the phase diagram calculation:

The screenshot shows the 'Calculation Type' settings in the TCAL8 software. The 'Phase diagram' option is selected with a radio button. Below it, there are three other options: 'Gibbs energy curves', 'Activity curves', and 'Phase fractions', each with a radio button and associated input fields for Temperature and Mole fraction. The 'Calculate Phase Diagram' button is highlighted with an arrow.

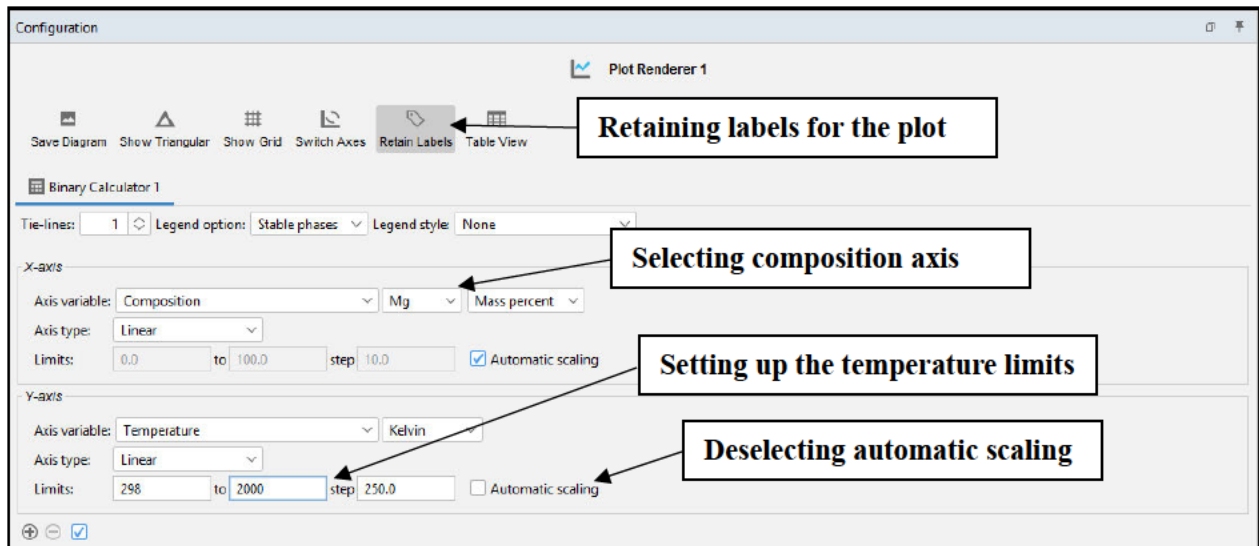
4. Choosing additional settings:

i) Phases and phase constitution



Status	Name ^	TCAL8
Entered	AL2CU_C16	<input checked="" type="checkbox"/>
Entered	AL2TI	<input checked="" type="checkbox"/>
Entered	AL2Y_C15	<input checked="" type="checkbox"/>
Entered	AL3CA8	<input checked="" type="checkbox"/>
Entered	AL3NI2	<input checked="" type="checkbox"/>
Entered	AL3TI_D022	<input checked="" type="checkbox"/>
Entered	AL3TI_LT	<input checked="" type="checkbox"/>
Entered	AL5TI2	<input checked="" type="checkbox"/>
Entered	AL7CU4NI	<input checked="" type="checkbox"/>
Entered	AL8FE5	<input checked="" type="checkbox"/>
Entered	ALM3_A15	<input checked="" type="checkbox"/>
Entered	ALMGZ_N_PHI	<input checked="" type="checkbox"/>
Entered	ALMG_BETA	<input checked="" type="checkbox"/>
Entered	ALMG_EPS	<input checked="" type="checkbox"/>
Entered	ALMG_GAMMA	<input checked="" type="checkbox"/>
Entered	ALT3_D019	<input checked="" type="checkbox"/>
Entered	AL7R2_B82	<input checked="" type="checkbox"/>
Entered	B2_BCC	<input checked="" type="checkbox"/>
Entered	B32_ALLI	<input checked="" type="checkbox"/>
Entered	BCC_B2	<input checked="" type="checkbox"/>

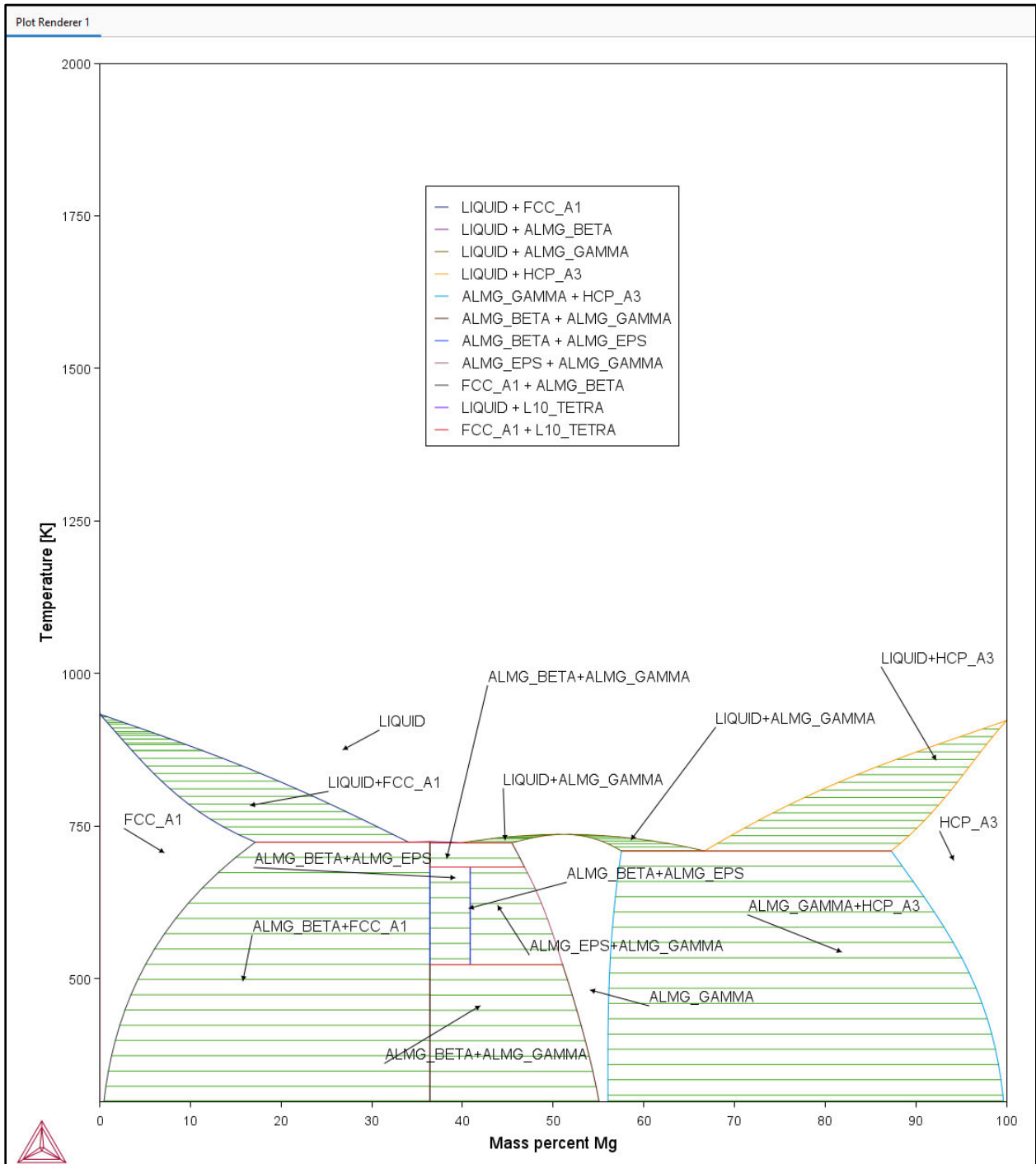
ii) Plot renderer configuration (Setting up the axes, and units and retaining the labels)



Configuration window for Plot Renderer 1. The interface includes a toolbar with options: Save Diagram, Show Triangular, Show Grid, Switch Axes, Retain Labels (highlighted with a callout box), and Table View. Below the toolbar, the 'Binary Calculator 1' section is visible, showing 'Tie-lines: 1', 'Legend option: Stable phases', and 'Legend style: None'. The X-axis configuration is set to 'Composition' (Mg) in 'Mass percent' units, with a linear axis type and limits from 0.0 to 100.0. The Y-axis configuration is set to 'Temperature' in 'Kelvin' units, with a linear axis type and limits from 298 to 2000. Callout boxes highlight: 'Retaining labels for the plot' (pointing to the Retain Labels button), 'Selecting composition axis' (pointing to the X-axis variable dropdown), 'Setting up the temperature limits' (pointing to the Y-axis limits input), and 'Deselecting automatic scaling' (pointing to the unchecked Automatic scaling checkbox for the Y-axis).

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

Help | Add Predecessor | Perform | Create New Successor

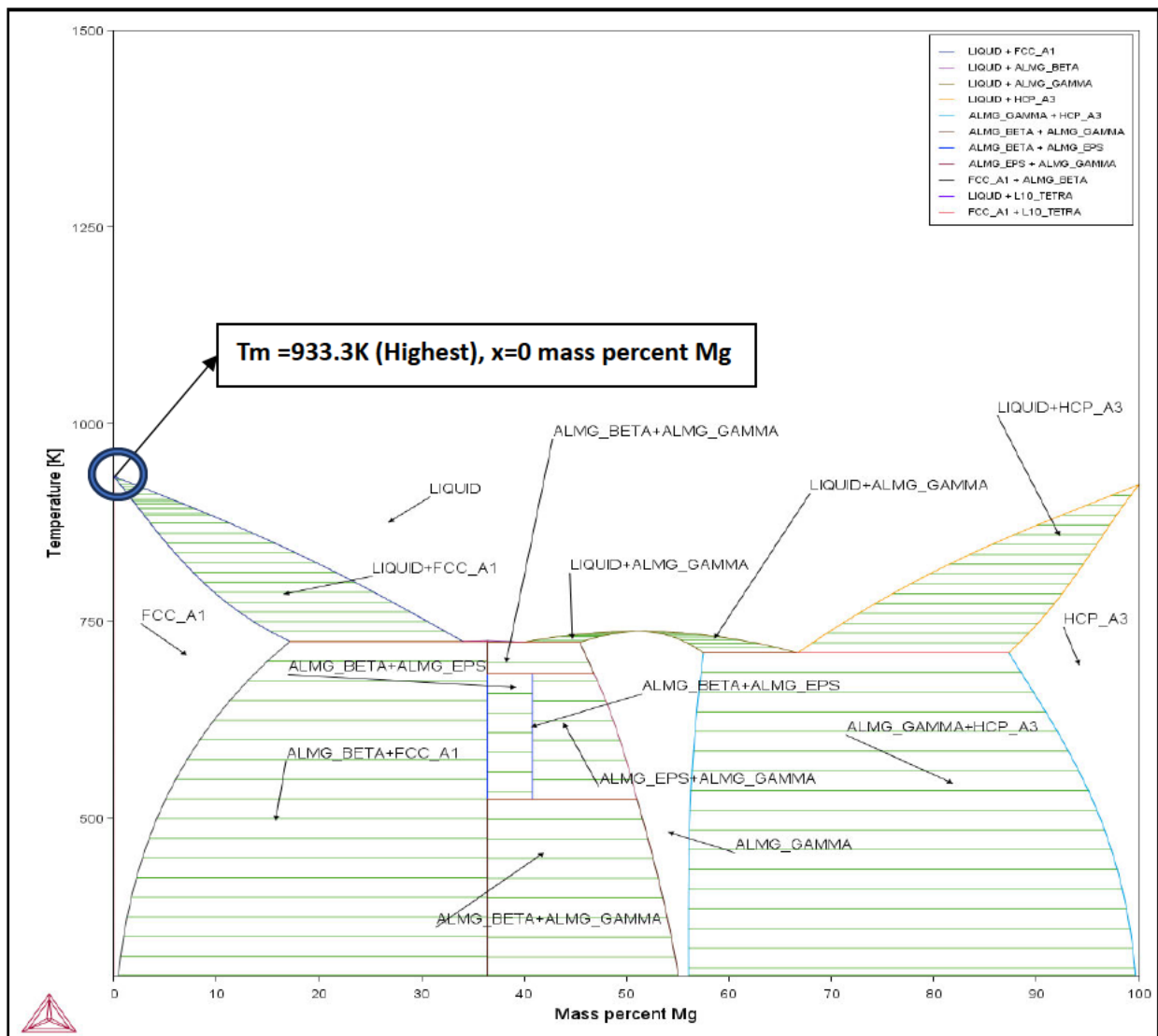


The labels in the above phase diagram were selected by right-clicking on the phase to be labeled and then selecting – “Add label”.

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.

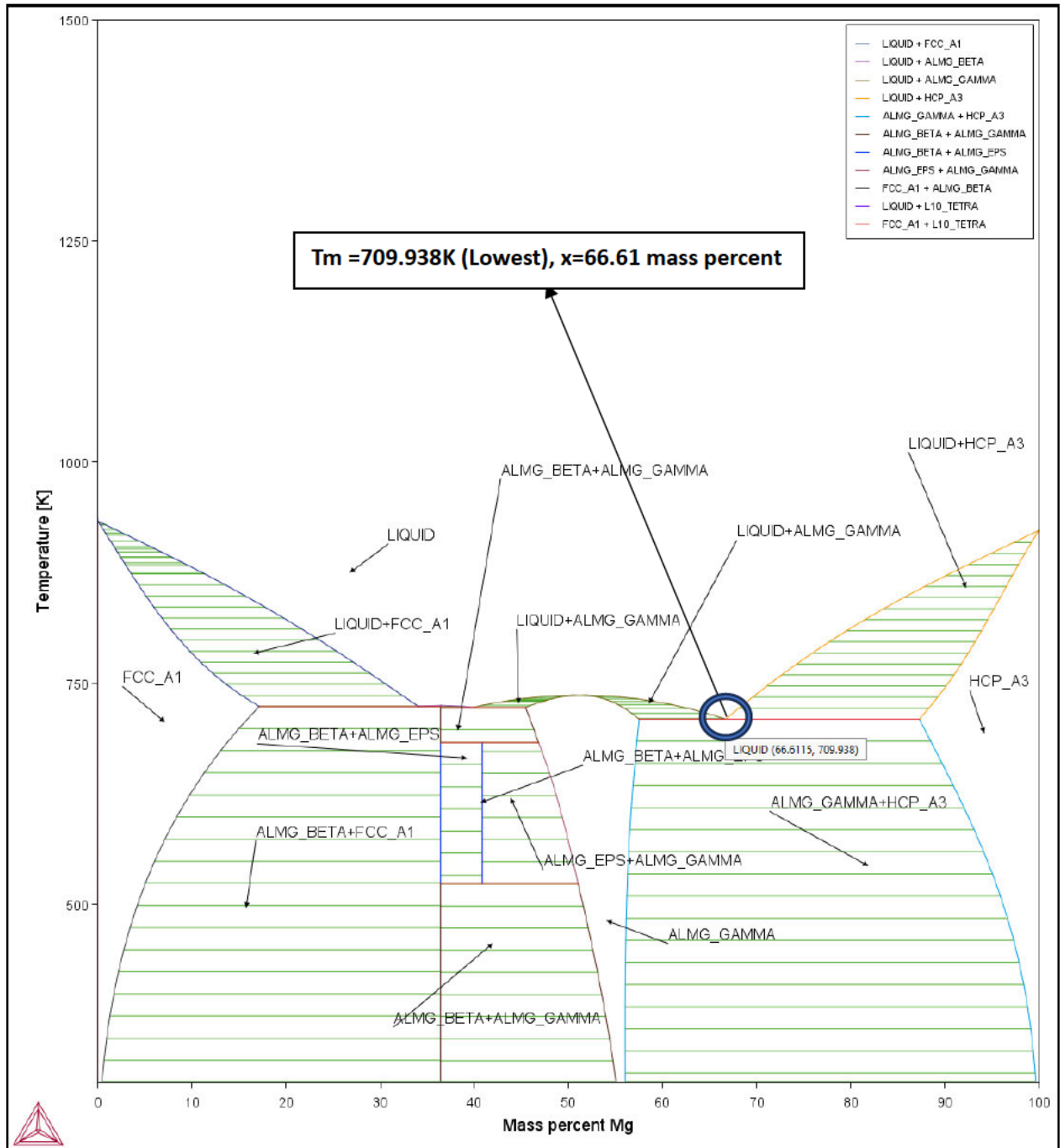
(c) Highest melting point and corresponding composition:

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.



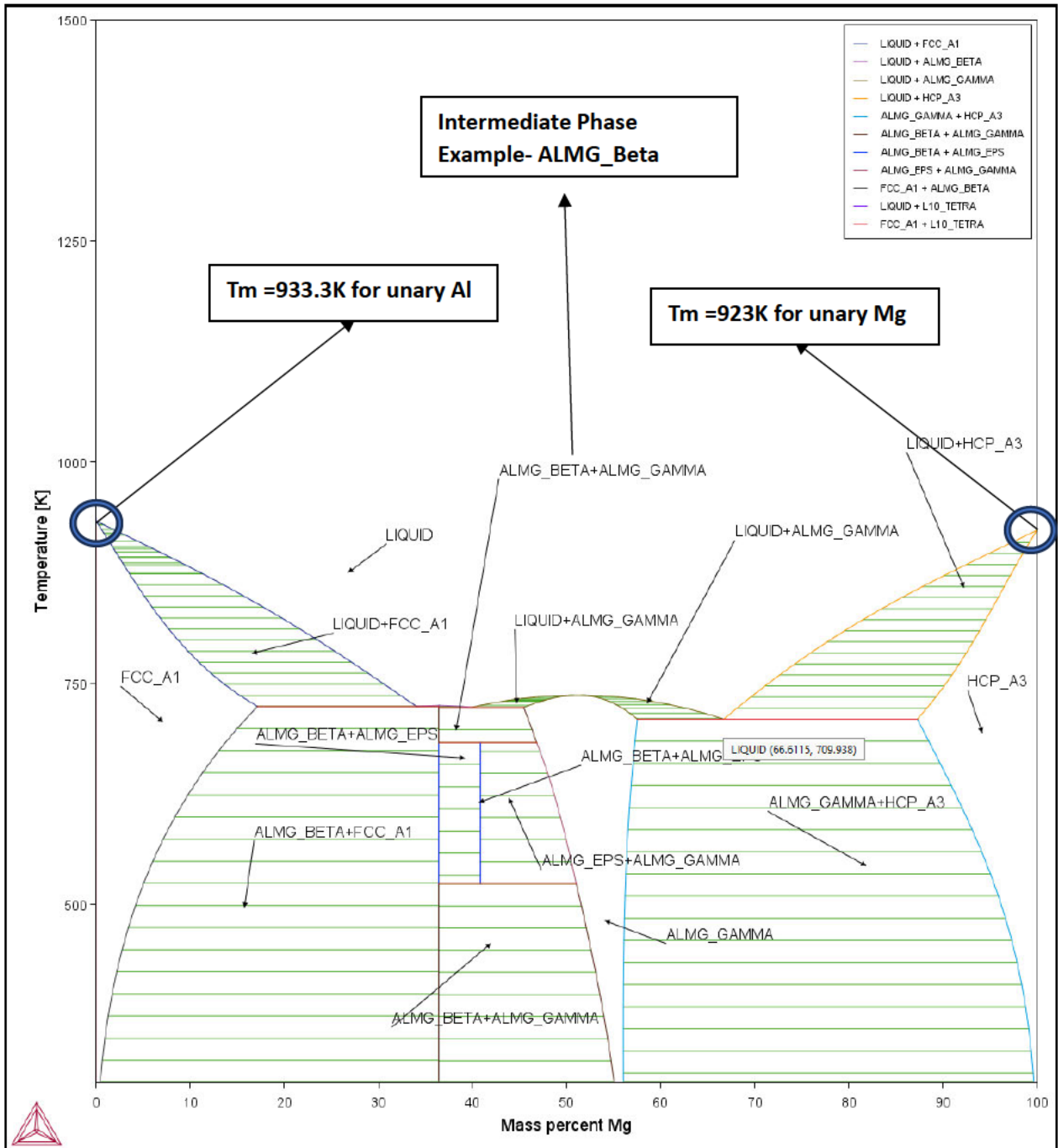
Lowest melting point and corresponding composition:

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.

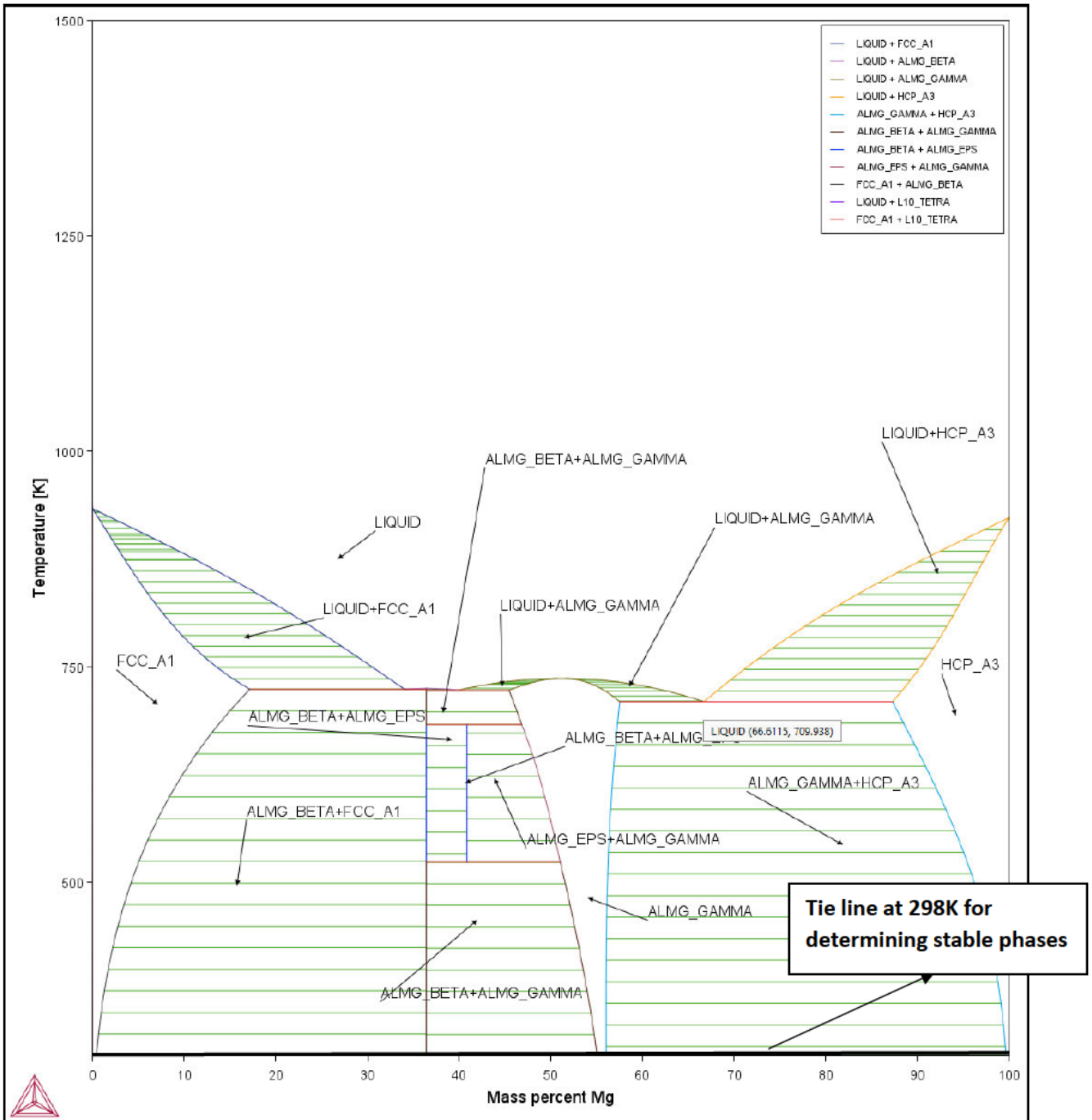


(d) Intermediate phases in the phase diagram

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.

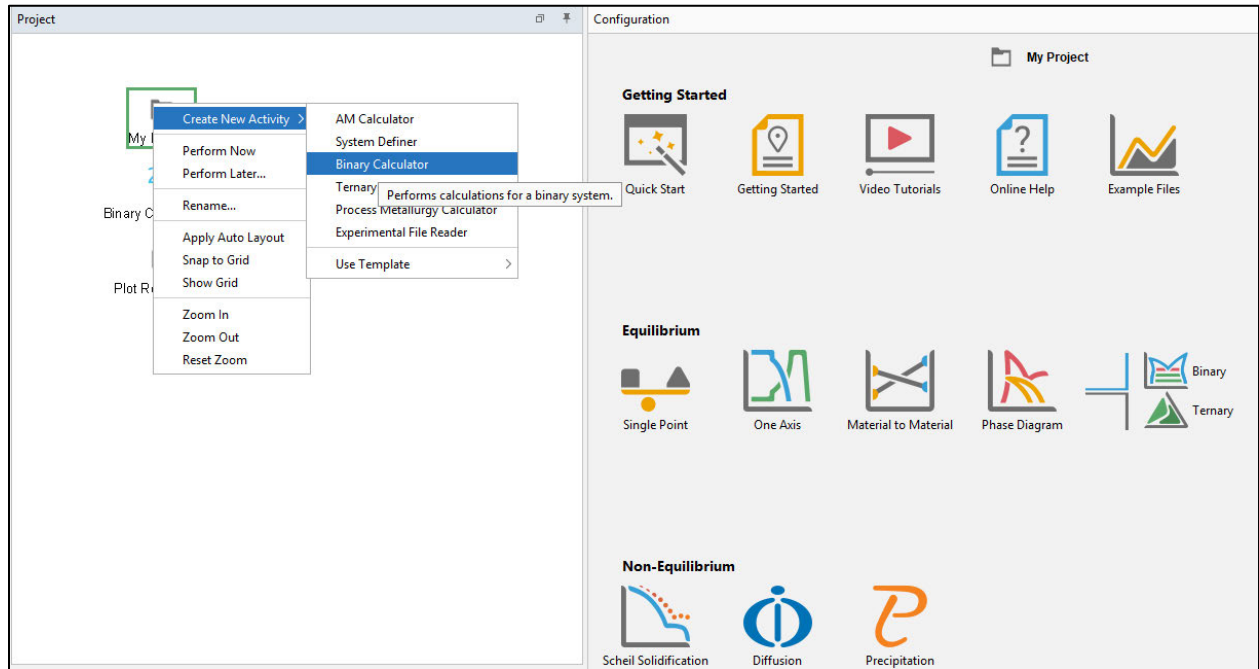
(e) Stable phases for unary systems at room temperature

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

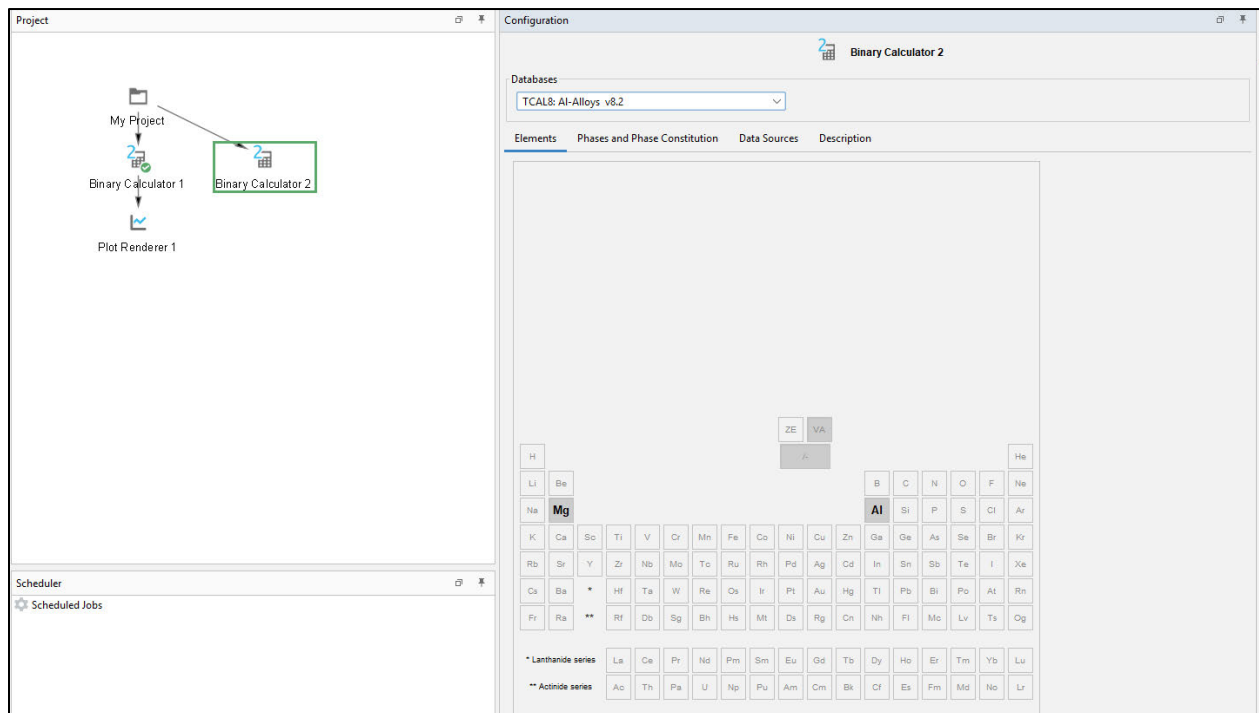


II. Calculation of Gibbs Free Energy

(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., $T=933.3\text{K}$) for the Gibbs free energy curves option in the GUI mode.

The screenshot displays the software interface. On the left, a project tree shows a hierarchy: 'My Project' contains 'Binary Calculator 1', 'Binary Calculator 2', and 'Plot Renderer 1'. On the right, the 'Binary Calculator 2' configuration window is open. It features a 'Databases' dropdown set to 'TCAL8: Al-Alloys v8.2'. Below this are tabs for 'Elements', 'Phases and Phase Constitution', 'Data Sources', and 'Description'. A periodic table is shown with 'Mg' and 'Al' highlighted. At the bottom, the 'Calculation Type' section has 'Gibbs energy curves' selected, with a temperature of 933.3 Kelvin. Buttons for 'Help', 'Add Predecessor', 'Calculate Gibbs Energy Curves', and 'Create New Successor' are visible at the bottom of the configuration window.

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

This screenshot shows the same software interface as the previous one, but with a context menu open over the 'Binary Calculator 2' icon in the project tree. The menu options are: 'Create New Successor > Plot Renderer', 'Perform Now', 'Perform Later...', 'Rename...', 'Remove', 'Clone', 'Clone Tree', 'Apply Auto Layout', 'Snap to Grid', 'Show Grid', 'Zoom In', 'Zoom Out', and 'Reset Zoom'. The configuration window for 'Binary Calculator 2' remains open in the background, showing the same settings as before.

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

Configuration Binary Calculator 4

Databases: TCAL8: Al-Alloys v8.2

Elements | **Phases and Phase Constitution** | Data Sources | Description

Phases

Status	Name ^	TCAL8
Entered	C15_LAVES	<input type="checkbox"/>
Entered	C36_LAVES	<input type="checkbox"/>
Entered	CBCC_A12	<input type="checkbox"/>
Entered	CU15SI4_EPSILON	<input type="checkbox"/>
Entered	CUB_A13	<input type="checkbox"/>
Entered	CUZR2_C11B	<input type="checkbox"/>
Entered	DHCP	<input type="checkbox"/>
Entered	DIAMOND_A4	<input type="checkbox"/>
Entered	FCC_A1	<input checked="" type="checkbox"/>
Entered	FEZN_ZETA	<input type="checkbox"/>
Entered	GAS	<input type="checkbox"/>
Entered	HCP_A3	<input type="checkbox"/>
Entered	L10_TETRA	<input type="checkbox"/>
Entered	L12_FCC	<input type="checkbox"/>
Entered	LIQUID	<input checked="" type="checkbox"/>
Entered	MG24R5	<input type="checkbox"/>
Entered	MG2ZN3	<input type="checkbox"/>
Entered	MG3CE	<input type="checkbox"/>
Entered	MGZN	<input type="checkbox"/>
Entered	NIZN_LT	<input type="checkbox"/>
Entered	O1_DIS	<input type="checkbox"/>
Entered	T_PHASE	<input type="checkbox"/>
Entered	AG2CA	<input type="checkbox"/>
Entered	AG2ER	<input type="checkbox"/>
Entered	AG2LA	<input type="checkbox"/>
Entered	AG2NA	<input type="checkbox"/>
Entered	AG4SC	<input type="checkbox"/>
Entered	AG51ER14	<input type="checkbox"/>
Entered	AG51LA14	<input type="checkbox"/>
Entered	AG5LA	<input type="checkbox"/>
Entered	AG5ZN8	<input type="checkbox"/>
Entered	AG7CA2	<input type="checkbox"/>
Entered	AG9CA2	<input type="checkbox"/>
Entered	AGCA3	<input type="checkbox"/>
Entered	AGER	<input type="checkbox"/>
Entered	AGLA	<input type="checkbox"/>
Entered	AGMG3	<input type="checkbox"/>
Entered	AGMG4	<input type="checkbox"/>

Check/uncheck all Add composition set...

TCAL8

Phase

Calculation Type

Phase diagram

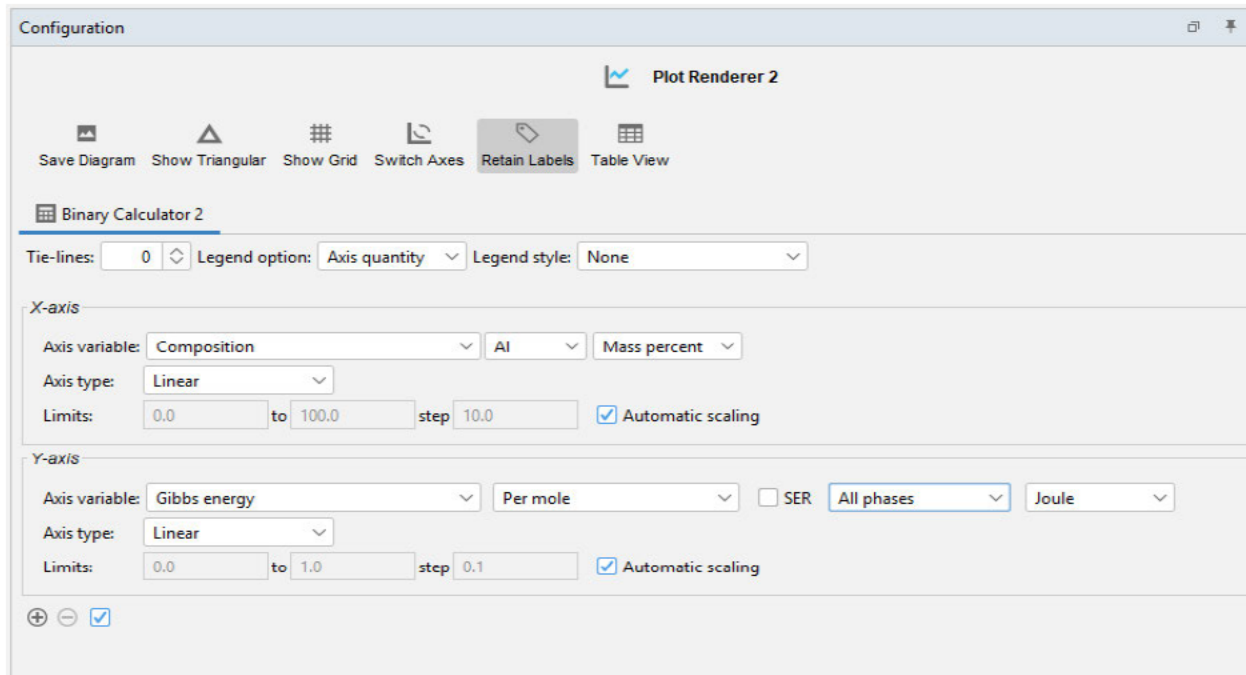
Gibbs energy curves Temperature

Activity curves Temperature

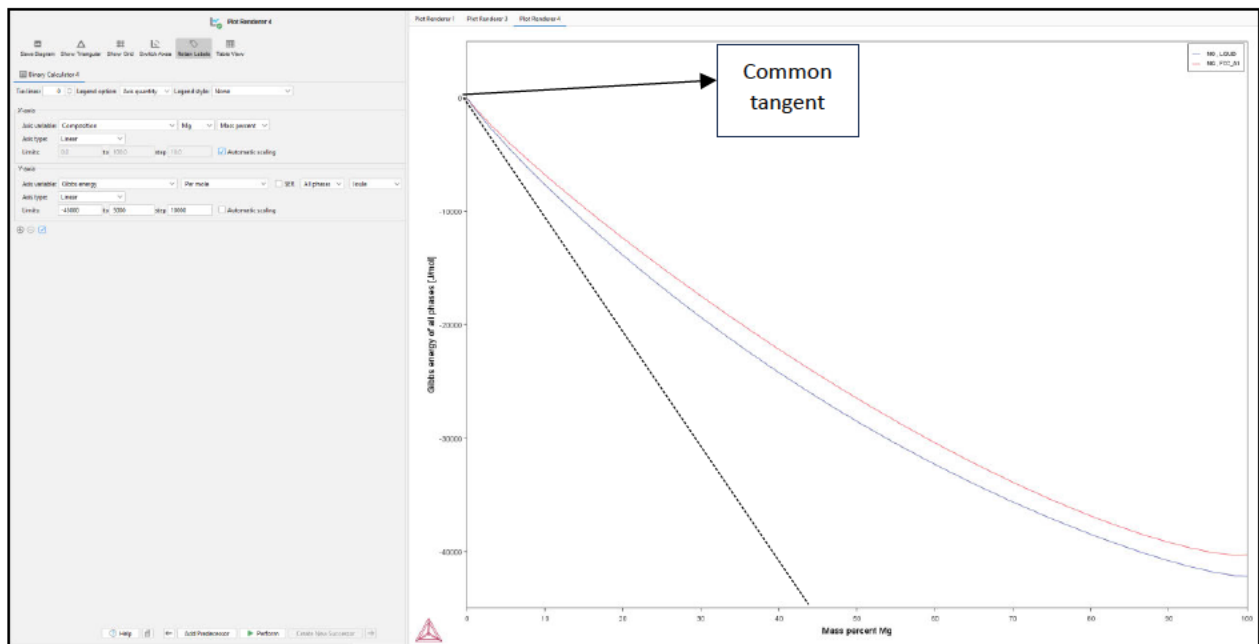
Phase fractions Mole fraction

Help ← Add Predecessor ▶ Calculate Gibbs Energy Curves Create New Successor →

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



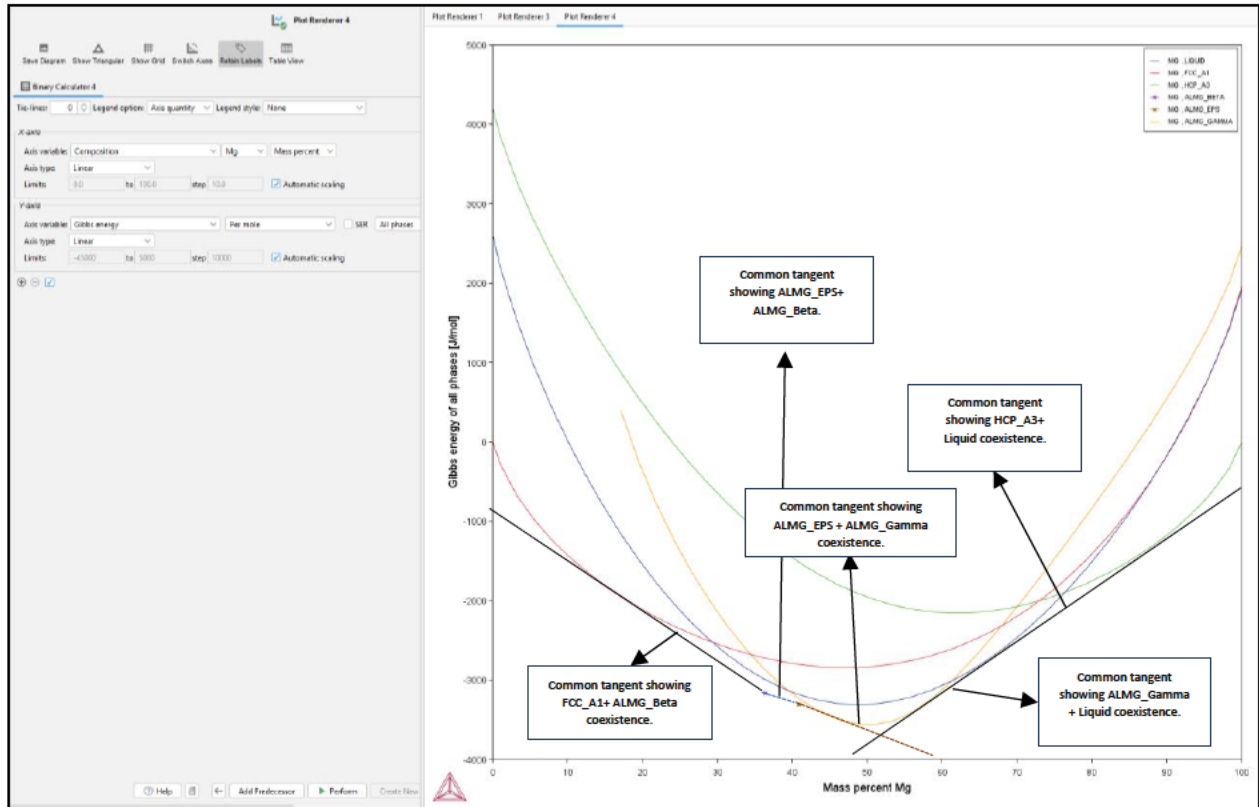
(b) G-X curves at the highest melting point ($T_m = 933.3\text{K}$)



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 ($T_m = 709.938\text{K}$)

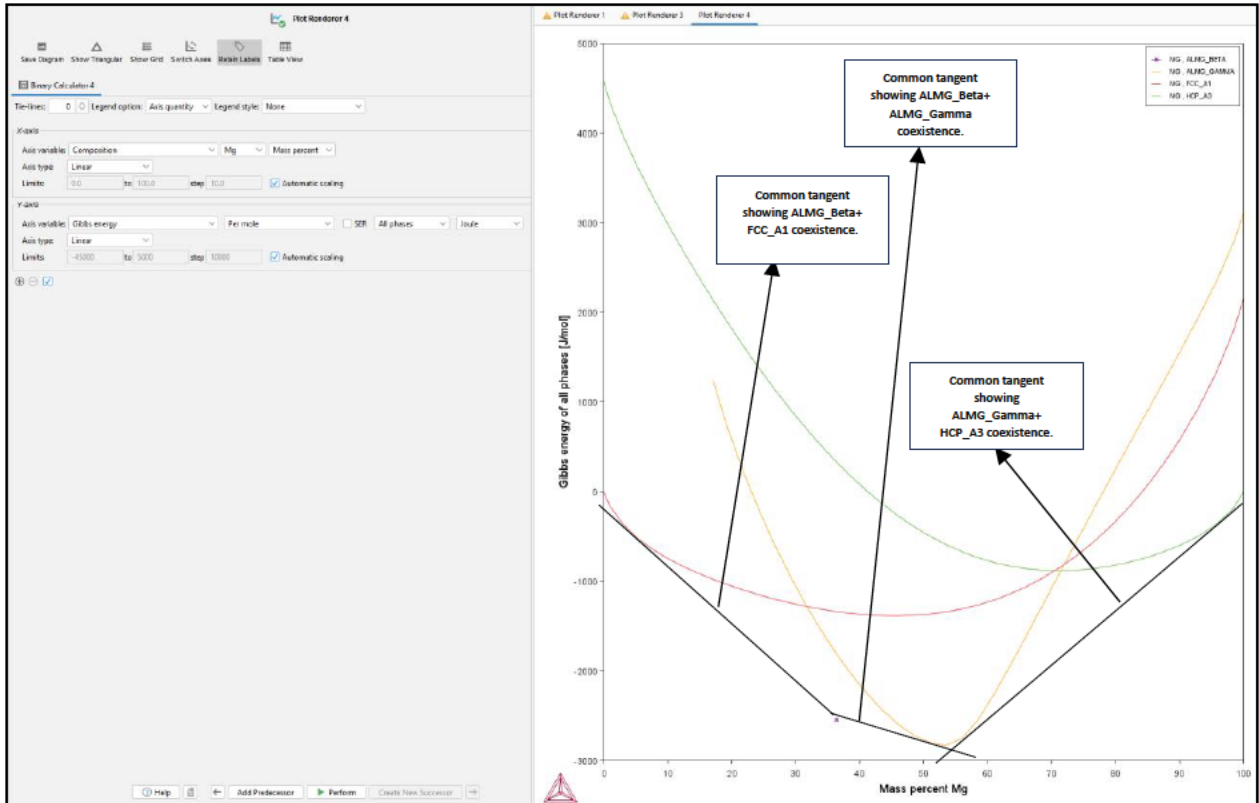
Stable phases/intermediates/compounds at $T = 709.938\text{K}$ according to the phase diagram: FCC_A1, ALMG_Beta, ALMG_EPS, Liquid, ALMG_Gamma, HCP_A3



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 ($T = 498\text{K}$)

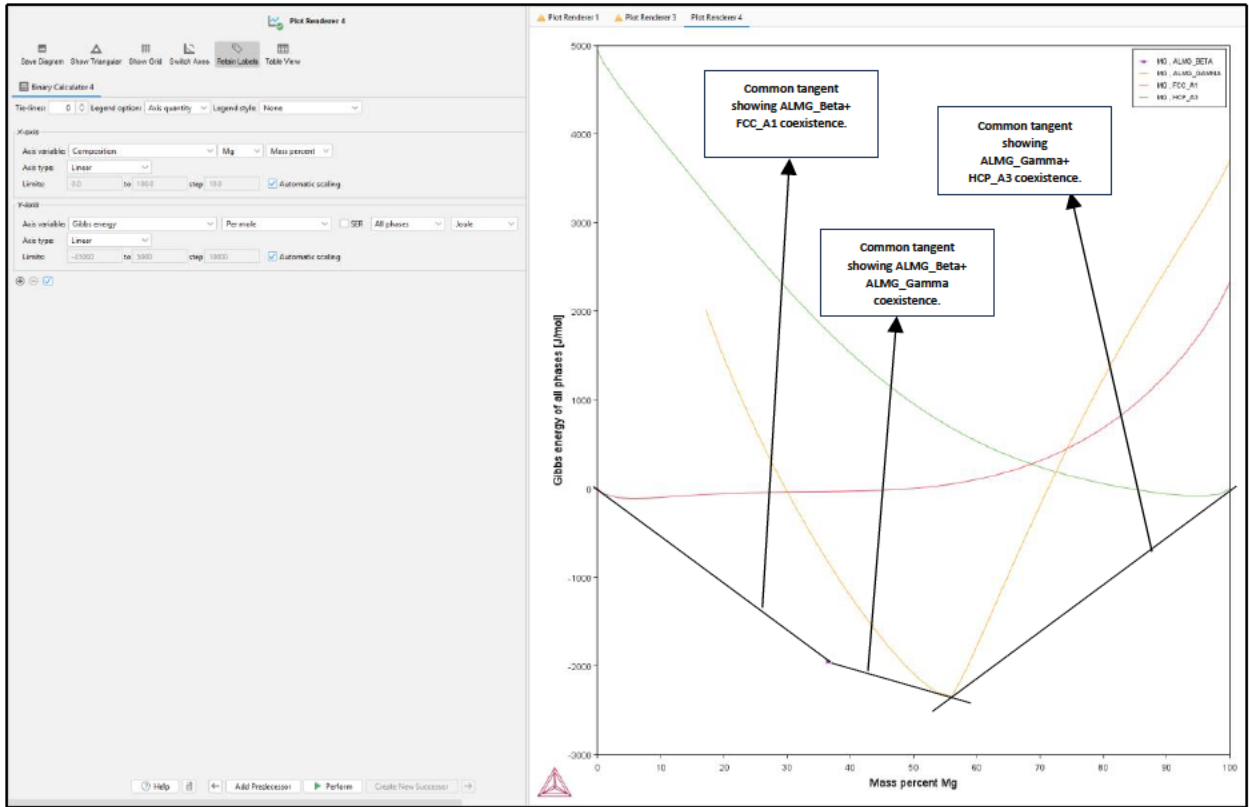
Stable phases/intermediates/compounds at $T = 498\text{K}$ according to the phase diagram: FCC_A1, ALMG_Beta, ALMG_Gamma, HCP_A3



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.

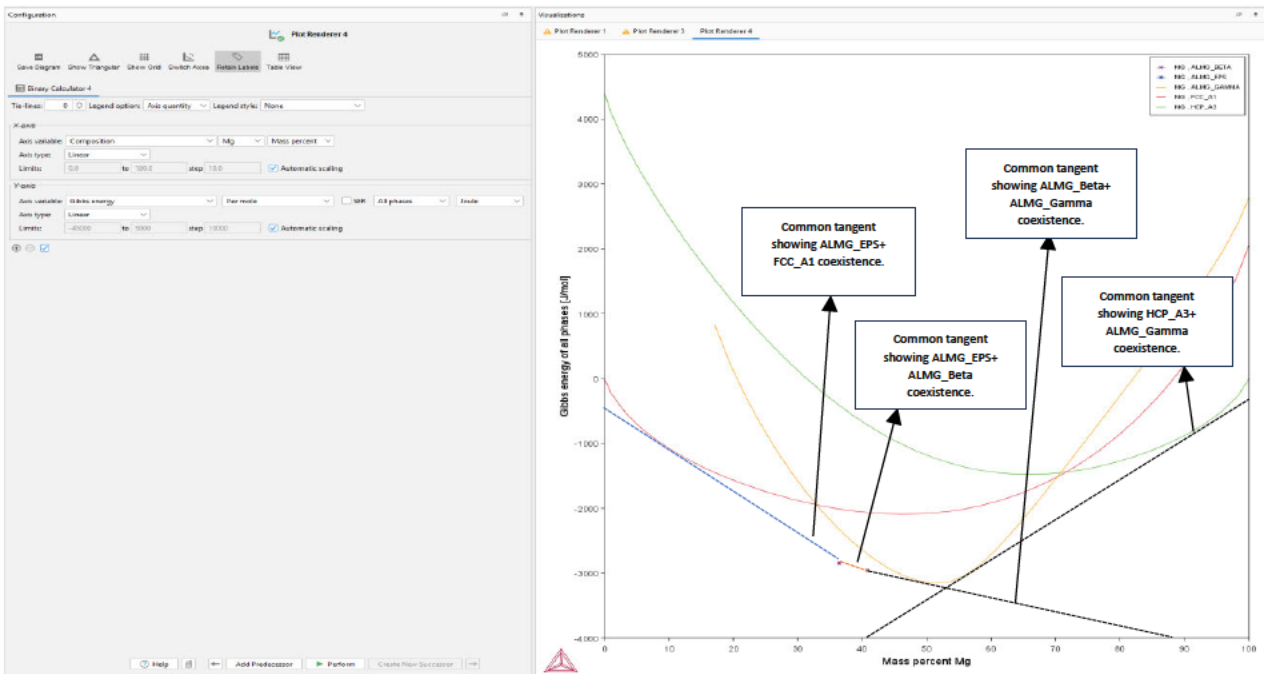
(e) G-X curves at room temperature (T= 298K)

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

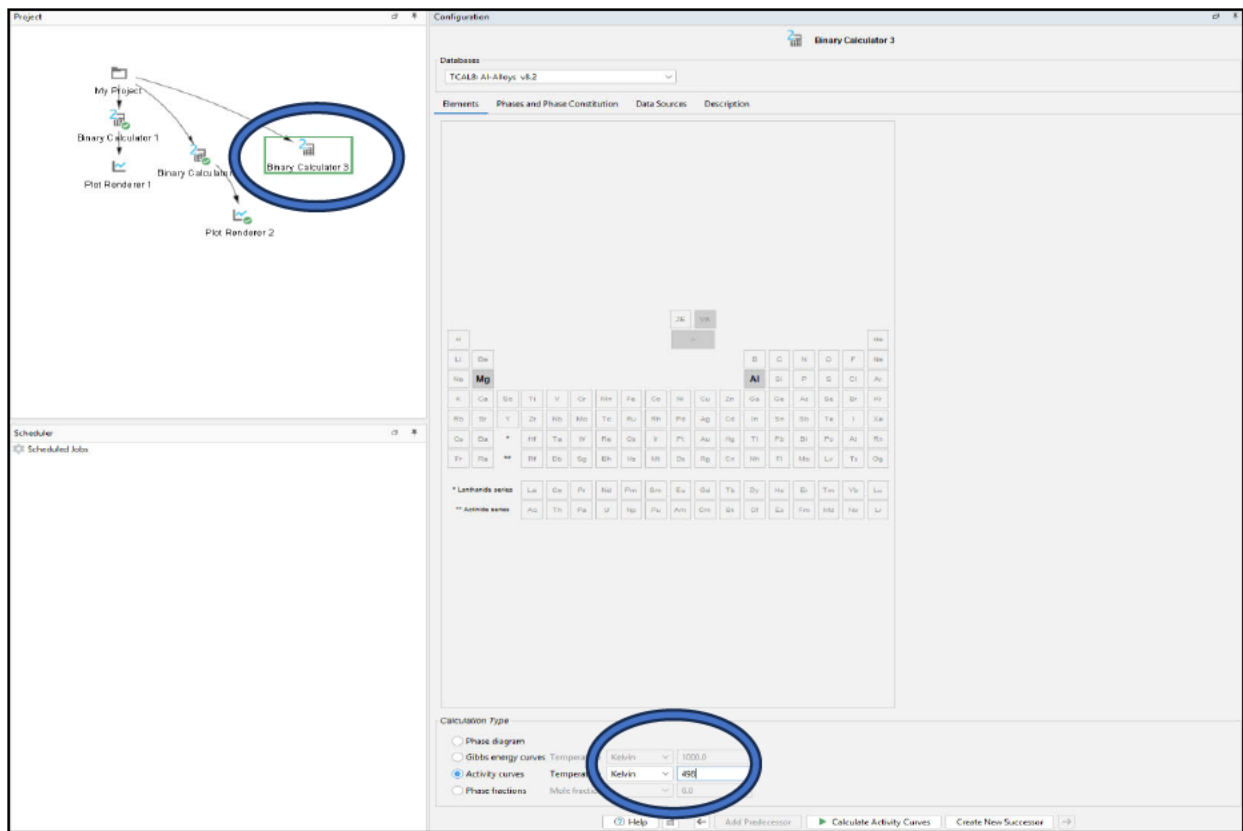
(a) At $T=498$ K, the stable phases according to the phase diagram are as follows: FCC_A1, ALMG_Gamma, and HCP_A3.

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.

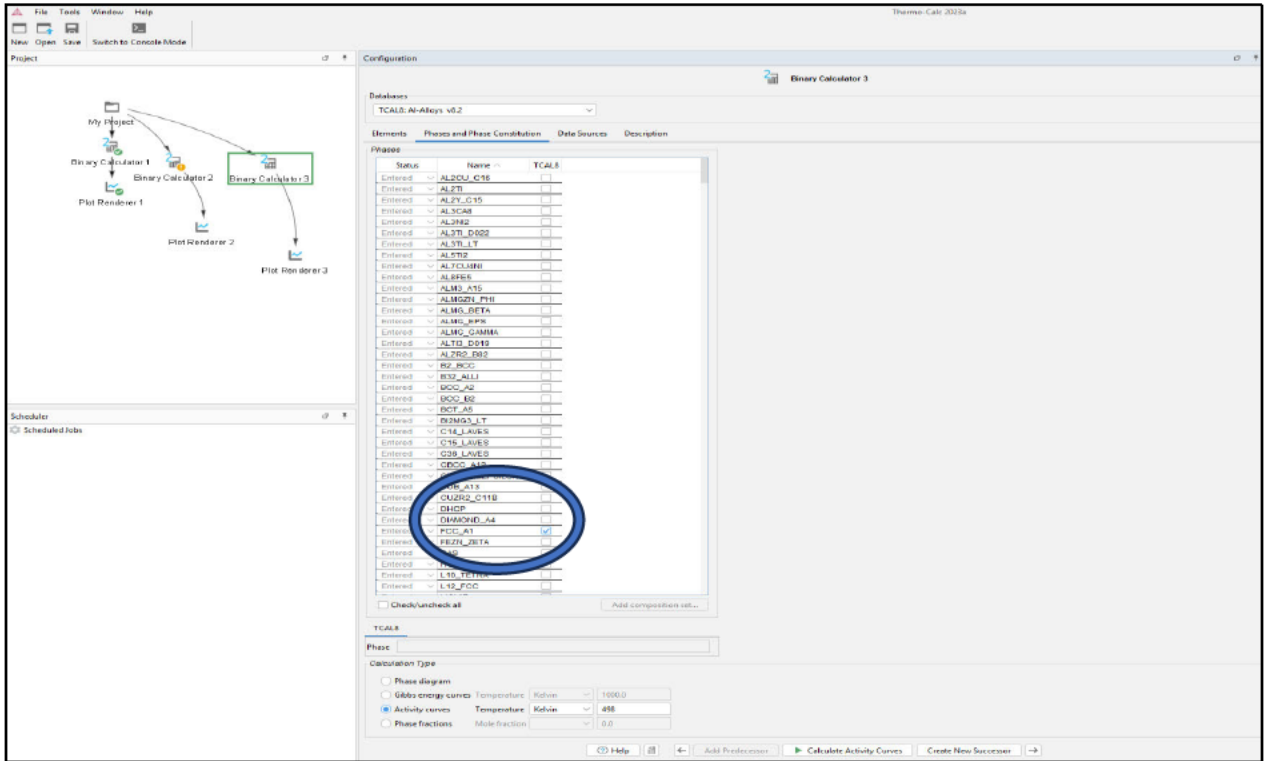
- **Activity of Al in FCC_A1**

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).

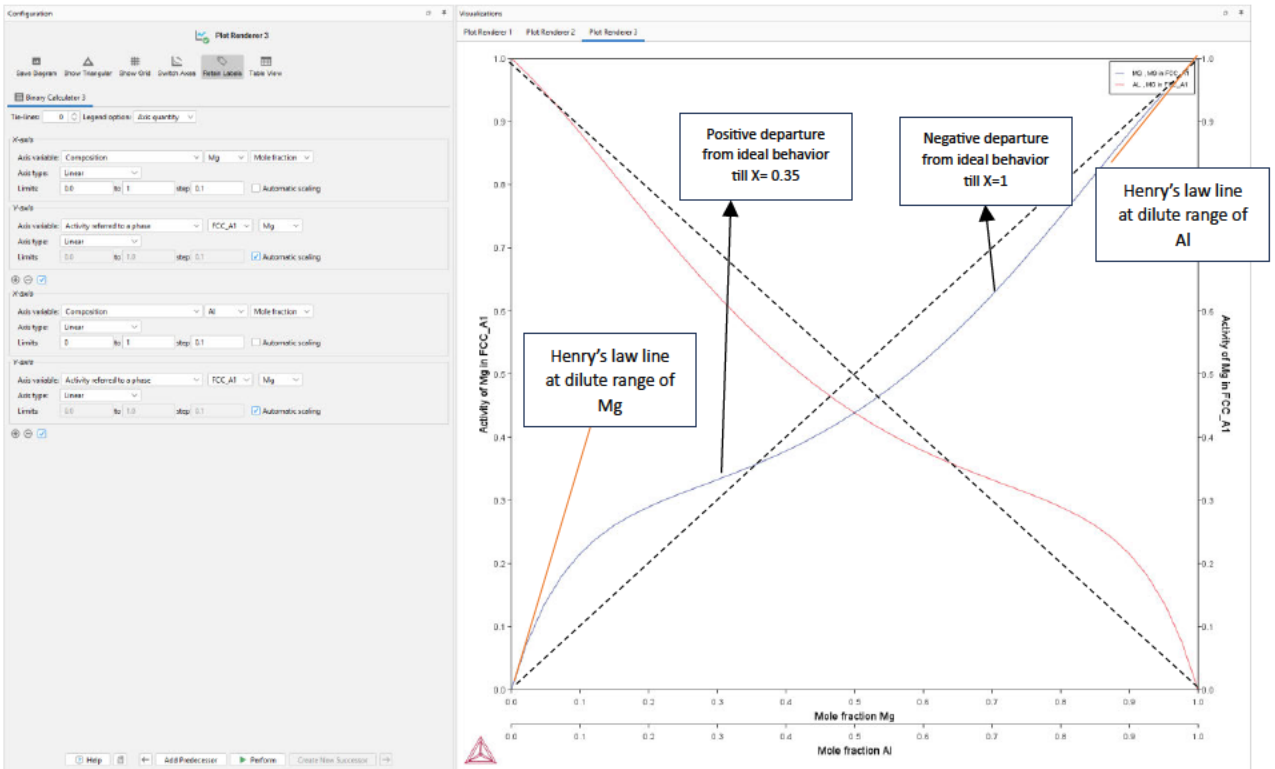


Step 2: Selecting the stable phases at the relevant temperature that were previously determined by drawing a tie line to the phase diagram at that temperature.

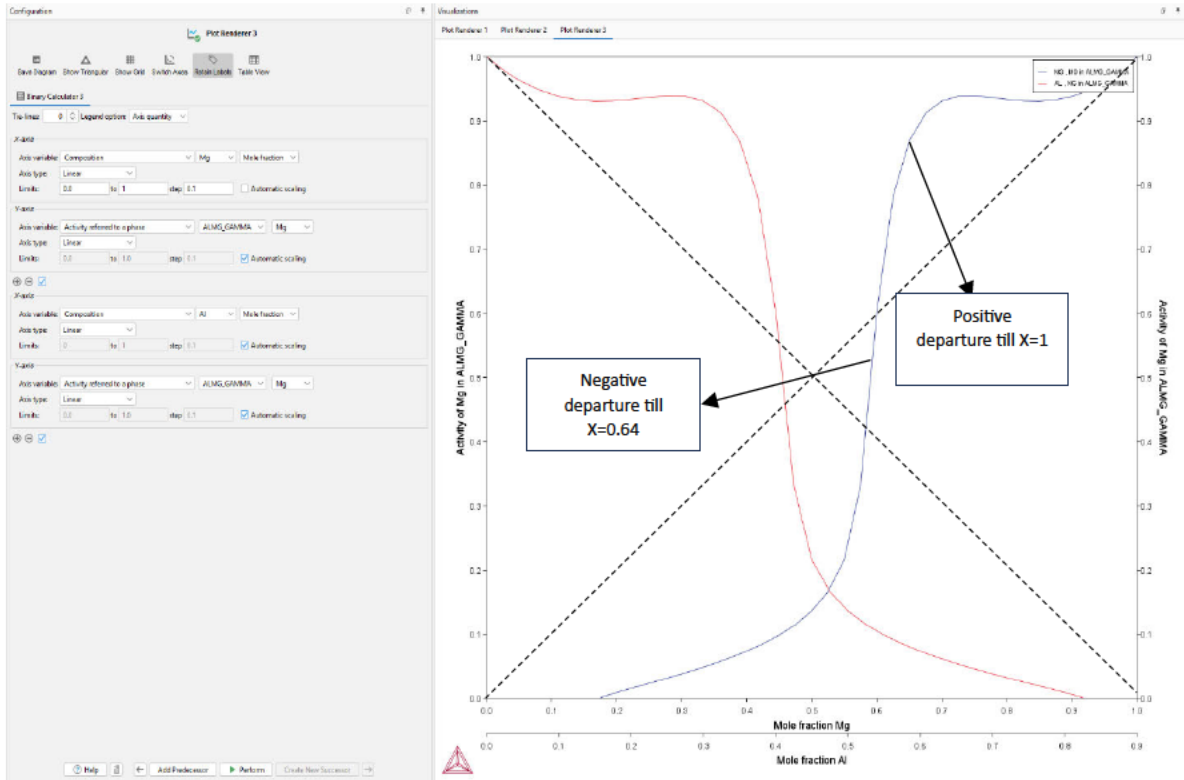


Step 3: Plotting the aX curve of the components in the stable phases

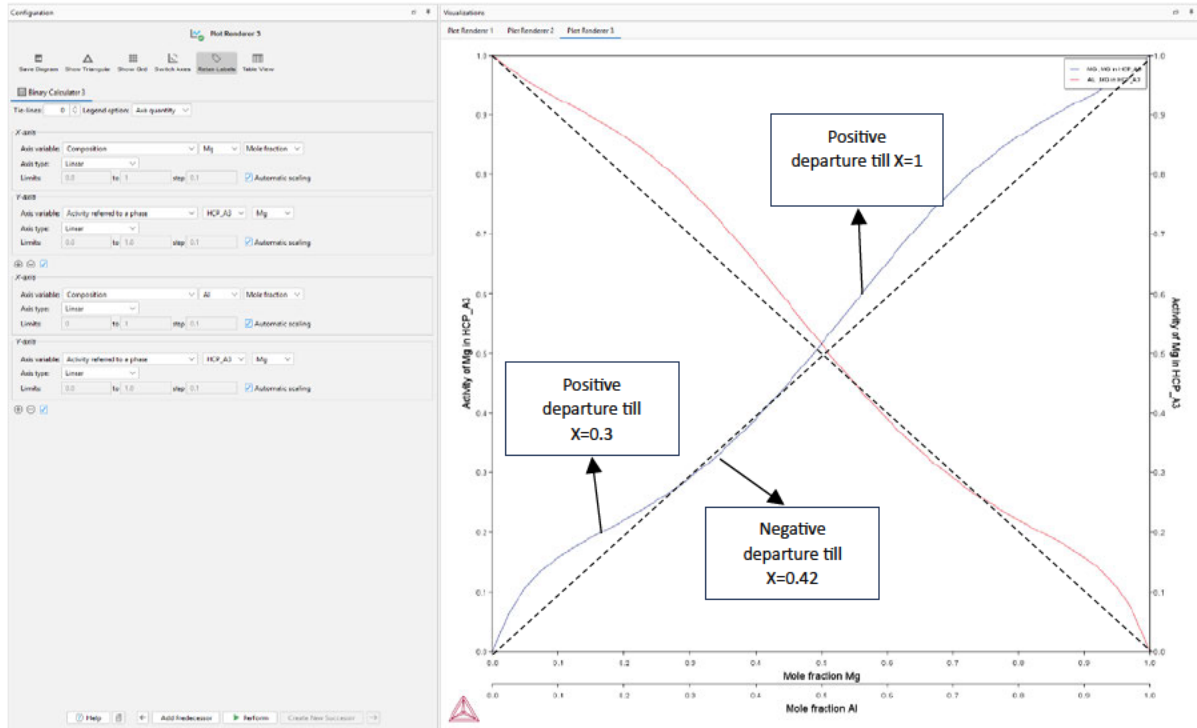
Mg in FCC_A1:



Mg in ALMG_Gamma:

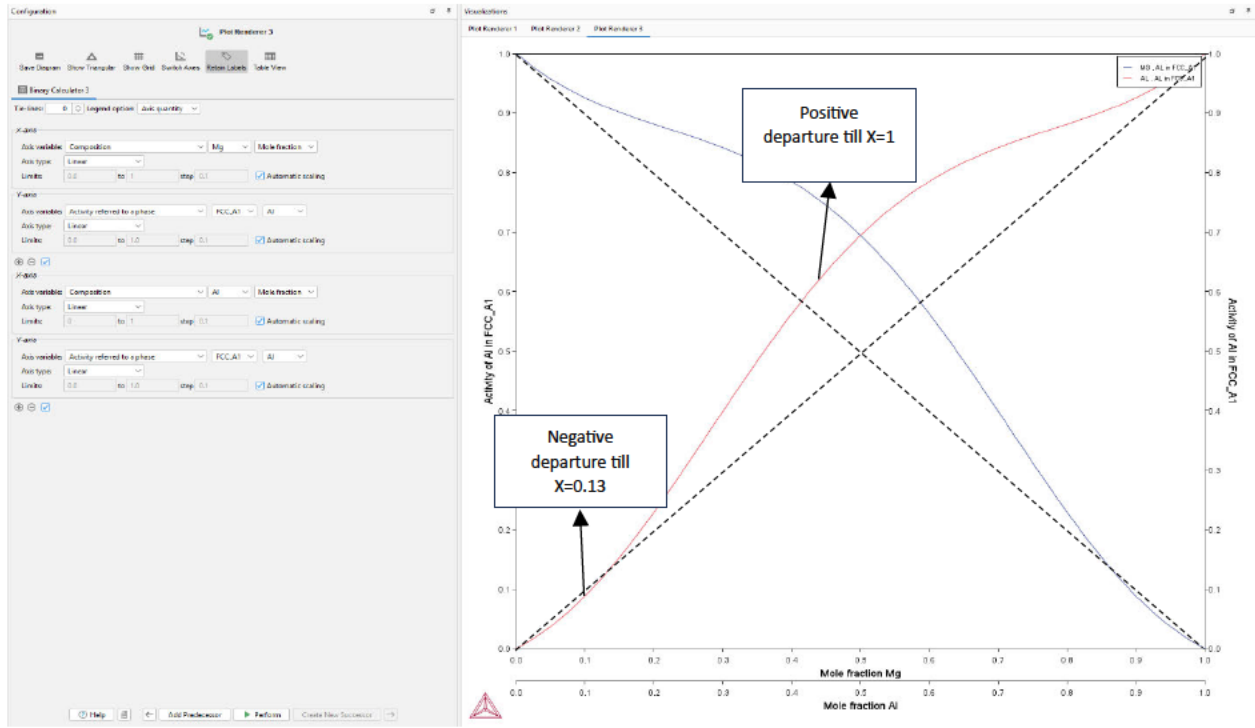


Mg in HCP_A3:

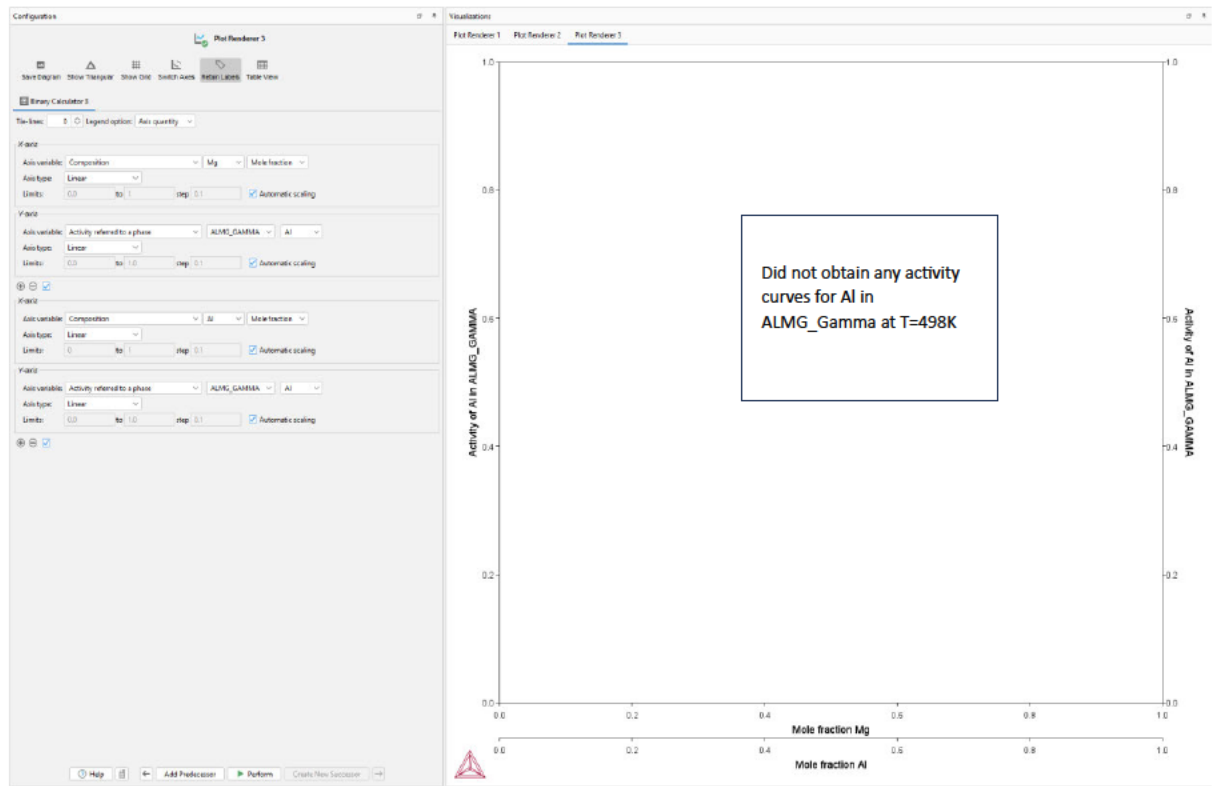


Step 4: Plotting the aX curve of Al in the stable phases

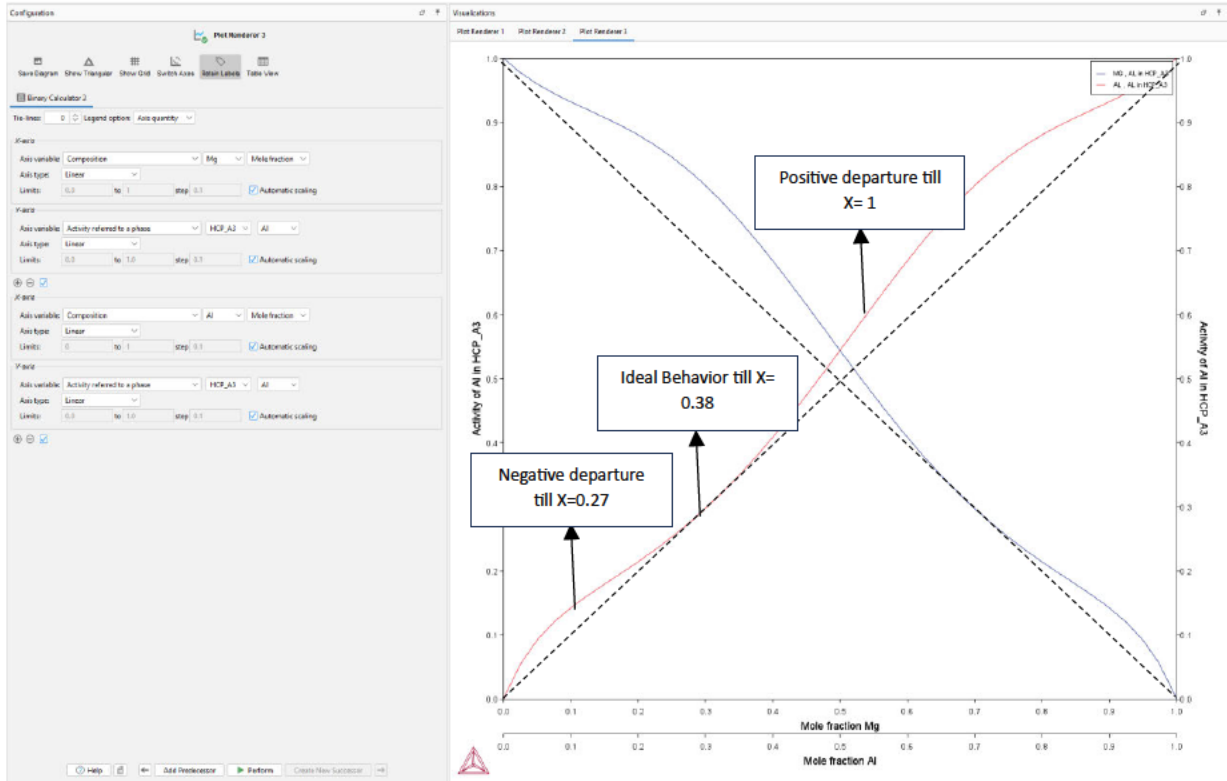
Al in FCC_A1:



Al in ALMG_Gamma:



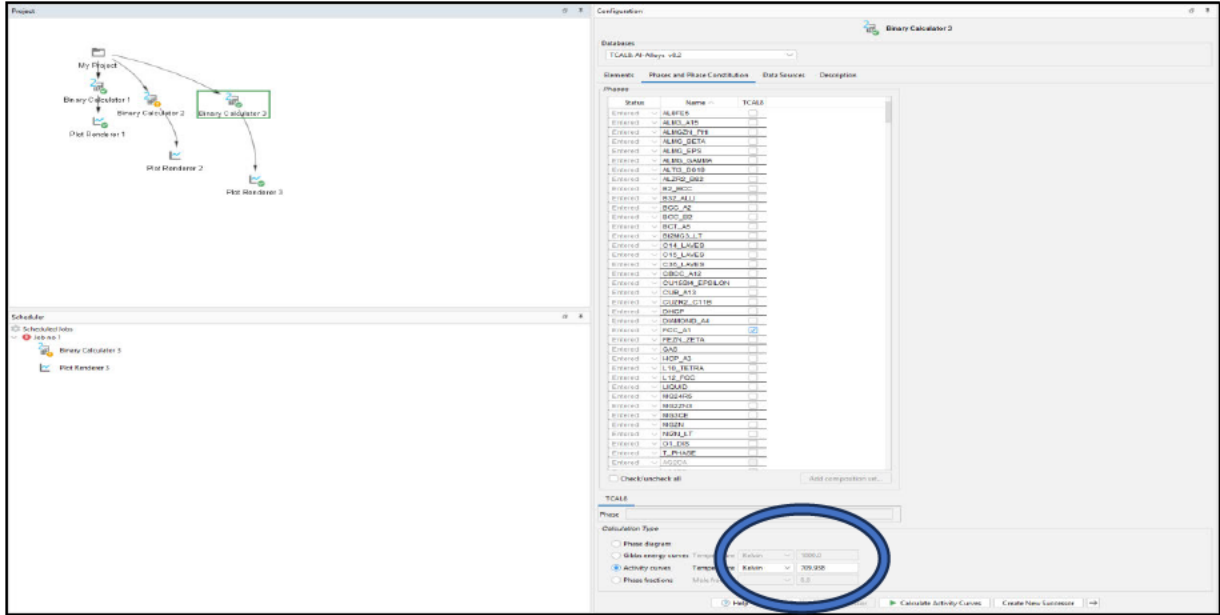
Al in HCP_A3:



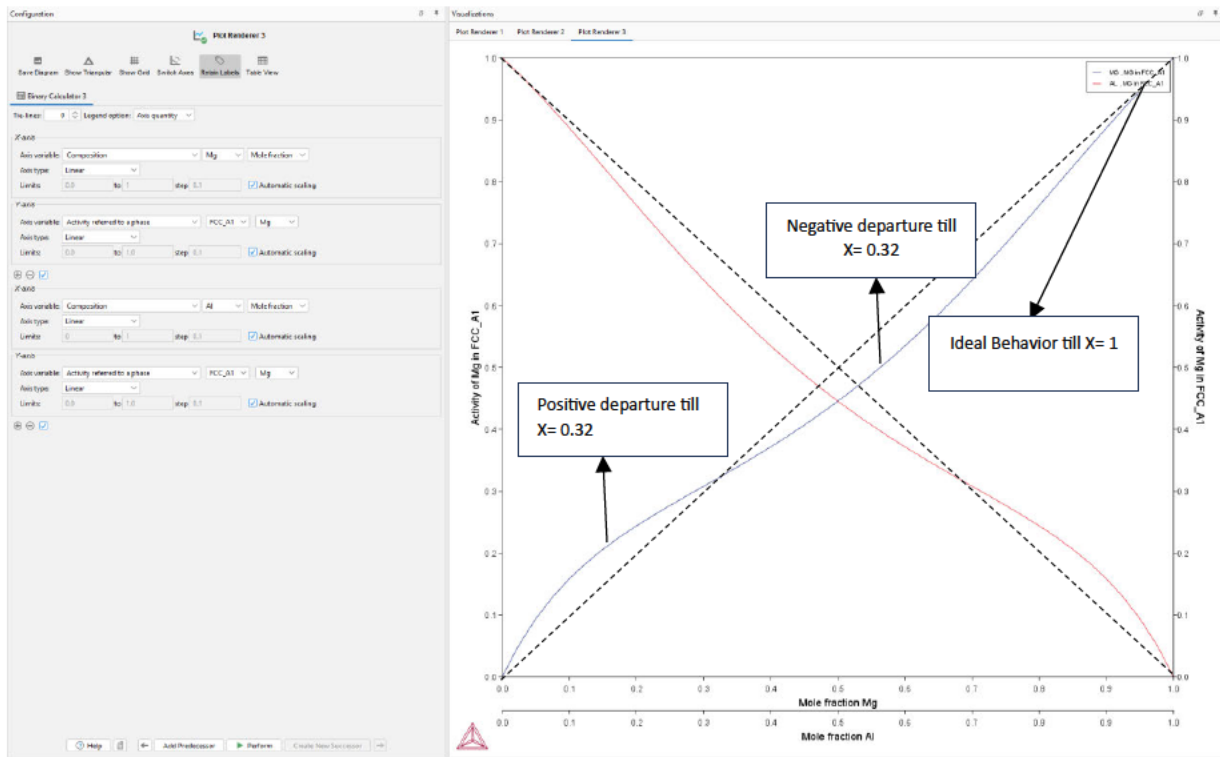
(b) At $T=709.938$ K, the stable phases according to the phase diagram are as follows:
FCC_A1, Liquid, ALMG_Gamma, and HCP_A3.

The ALMG_Beta and ALMG_EPS are vertical lines indicative of compounds.

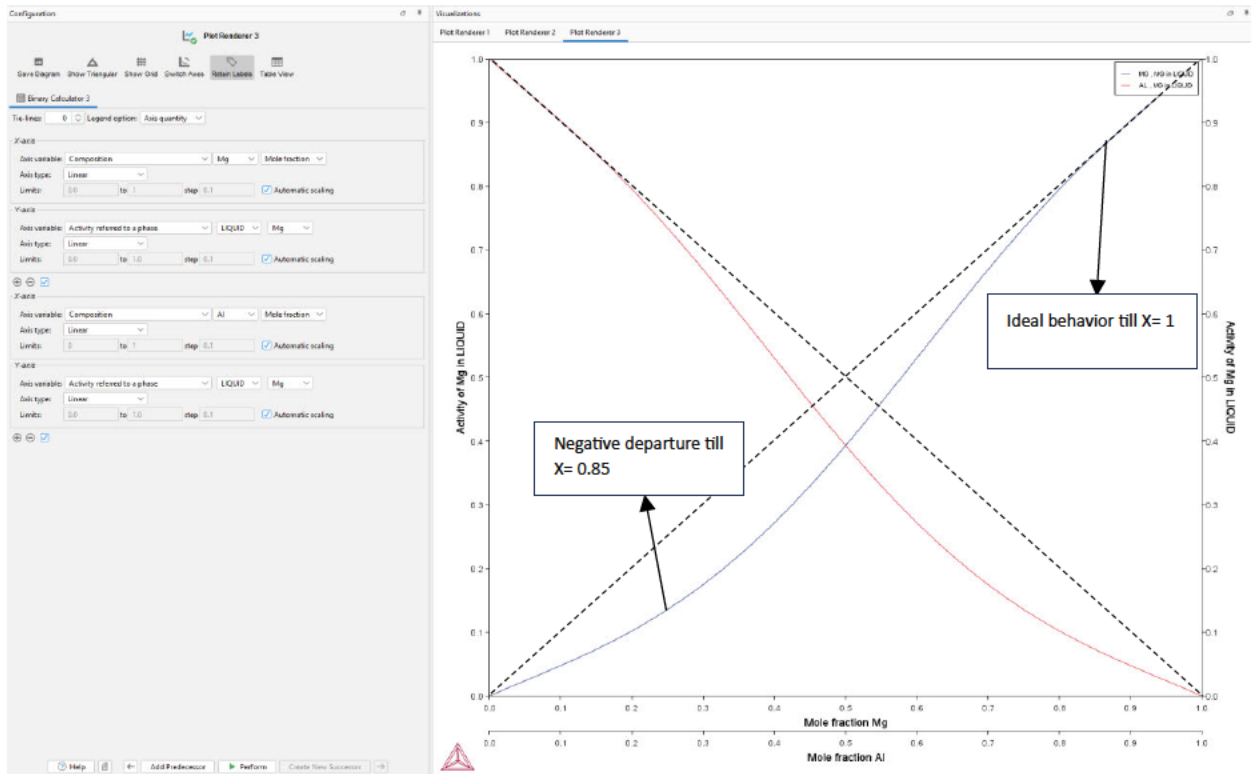
Calculation Step (Selecting lowest melting point temperature):



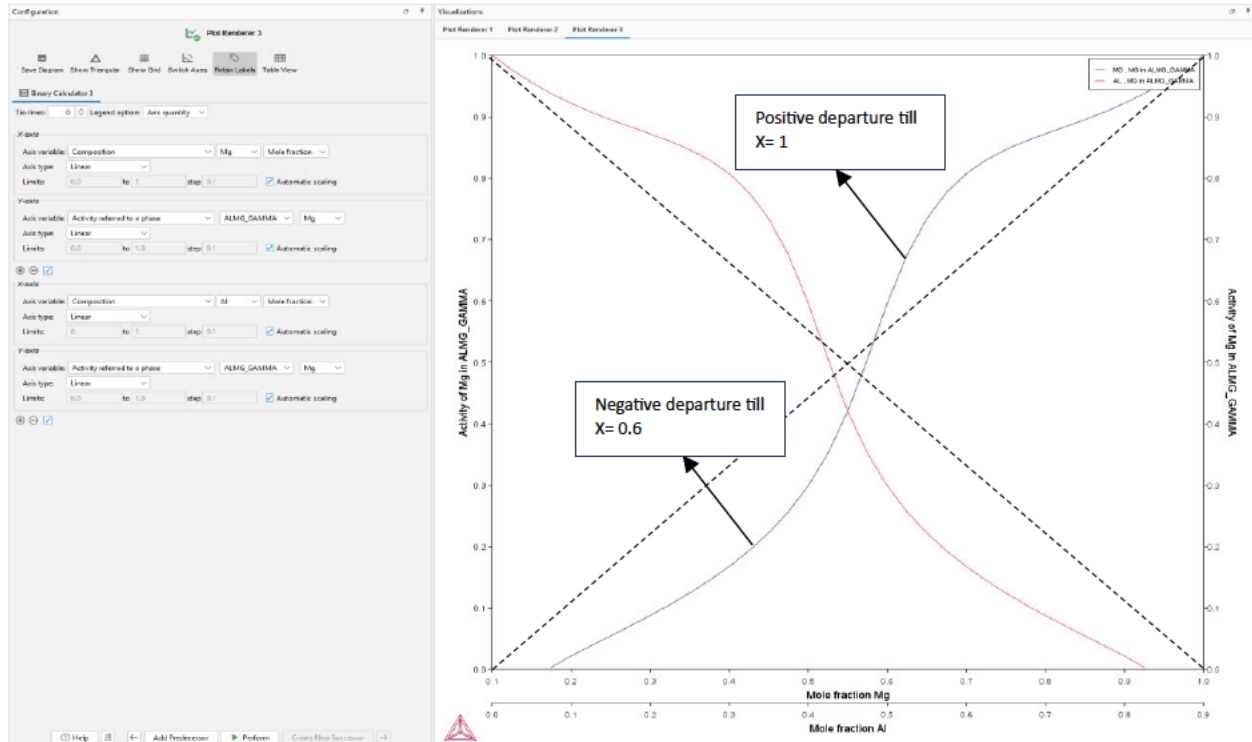
Mg in FCC_A1:



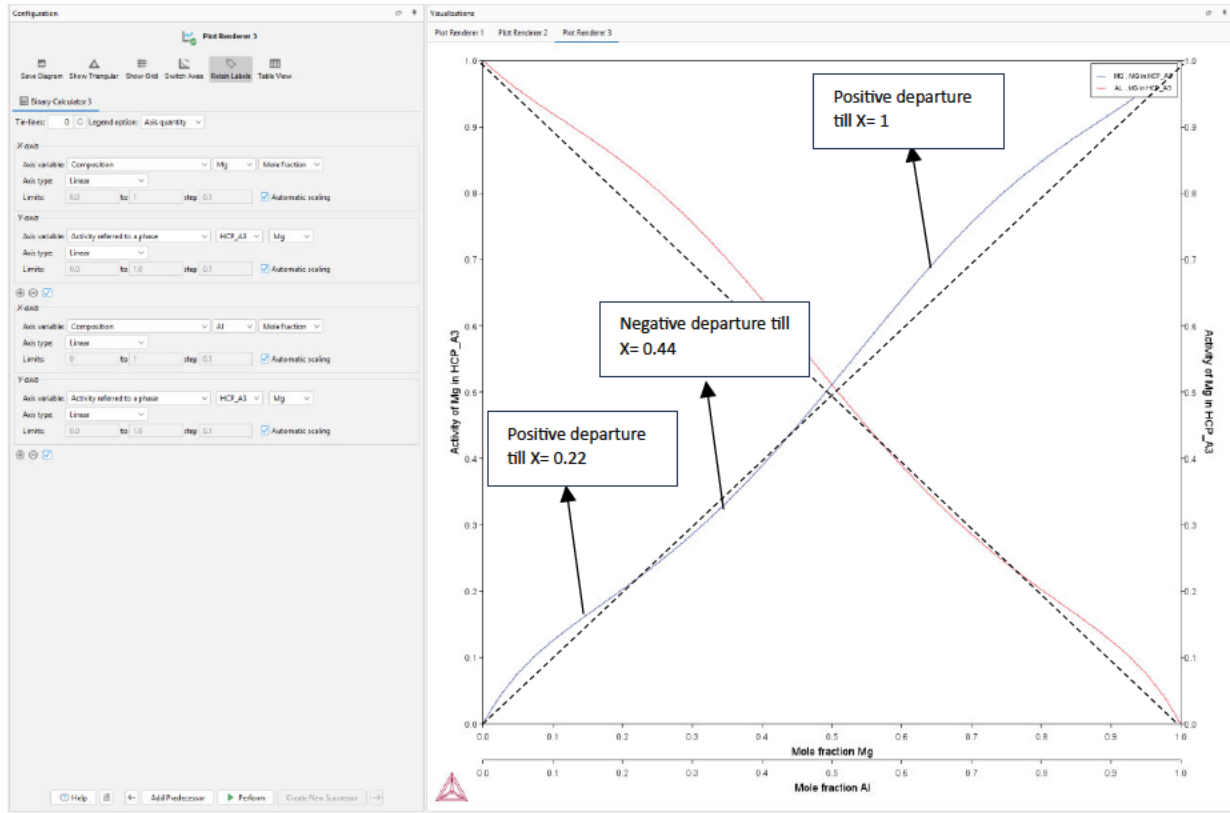
Mg in Liquid:



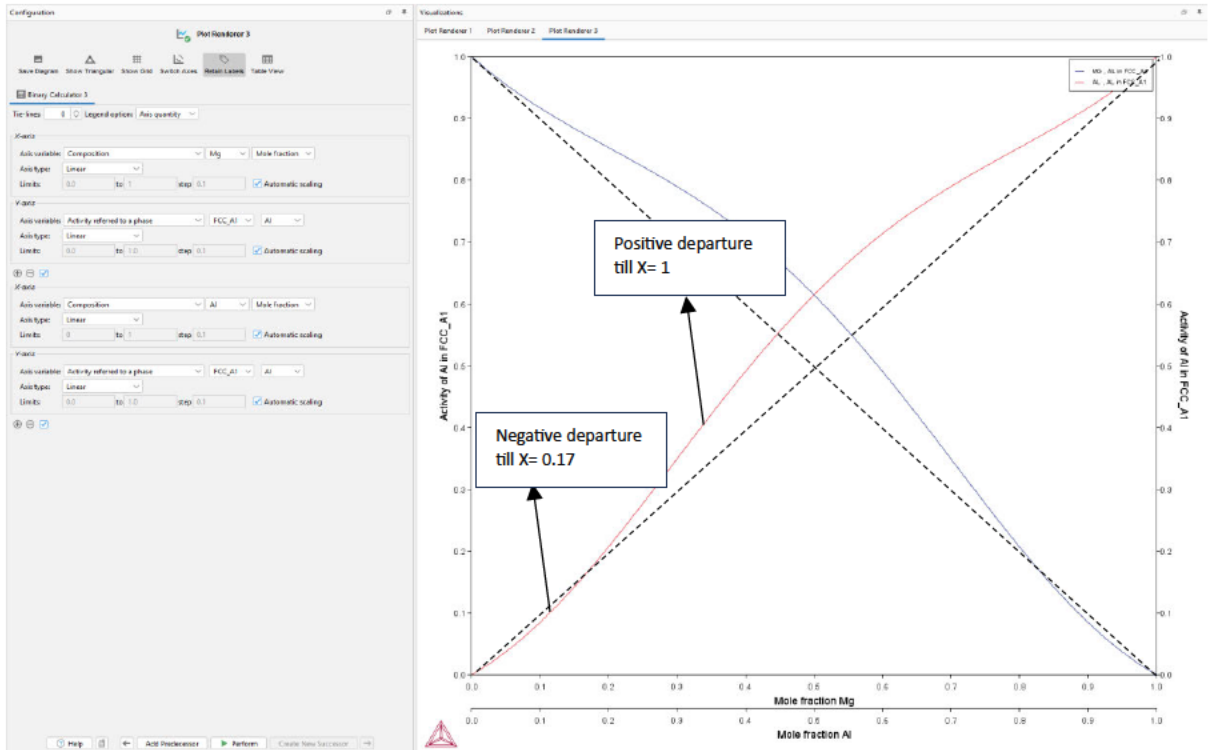
Mg in ALMG_Gamma:



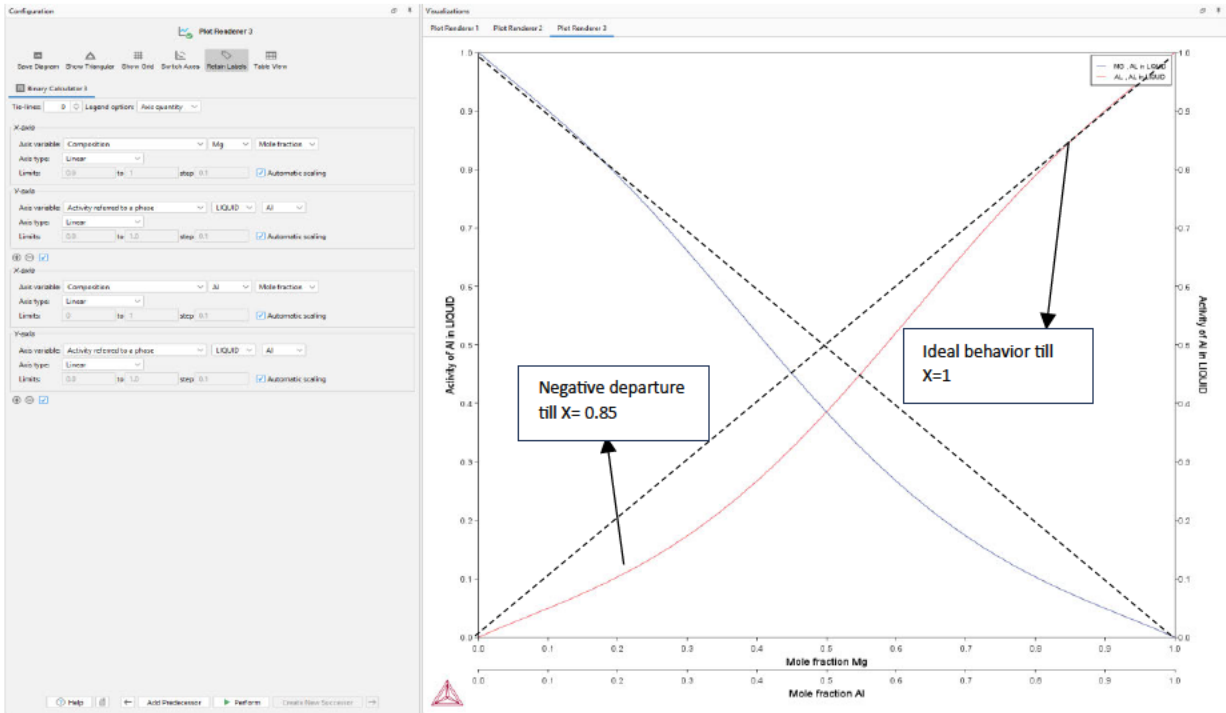
Mg in HCP_A3:



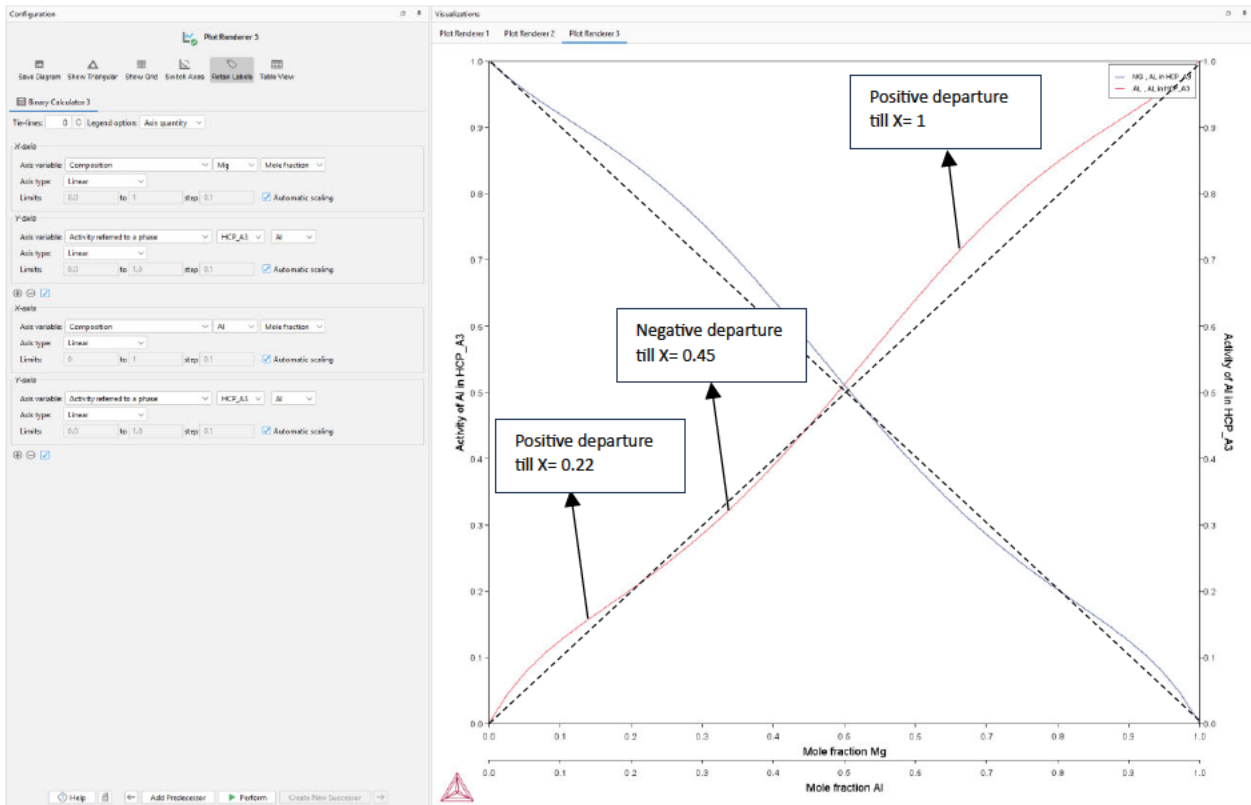
Al in FCC_A1:



Al in Liquid:



Al in HCP_A3:



References:

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