MATERIALS AND DESIGN

THERMO-CALC EXERCISE 1

Politecnico di Torino

1859

THERMO-CALC REPORT 1

NAMES	STUDENT ID
Siriro, Wiseman	S333263

POLYTECHNIC UNIVERSITY OF TURIN

ITALY

QUESTION

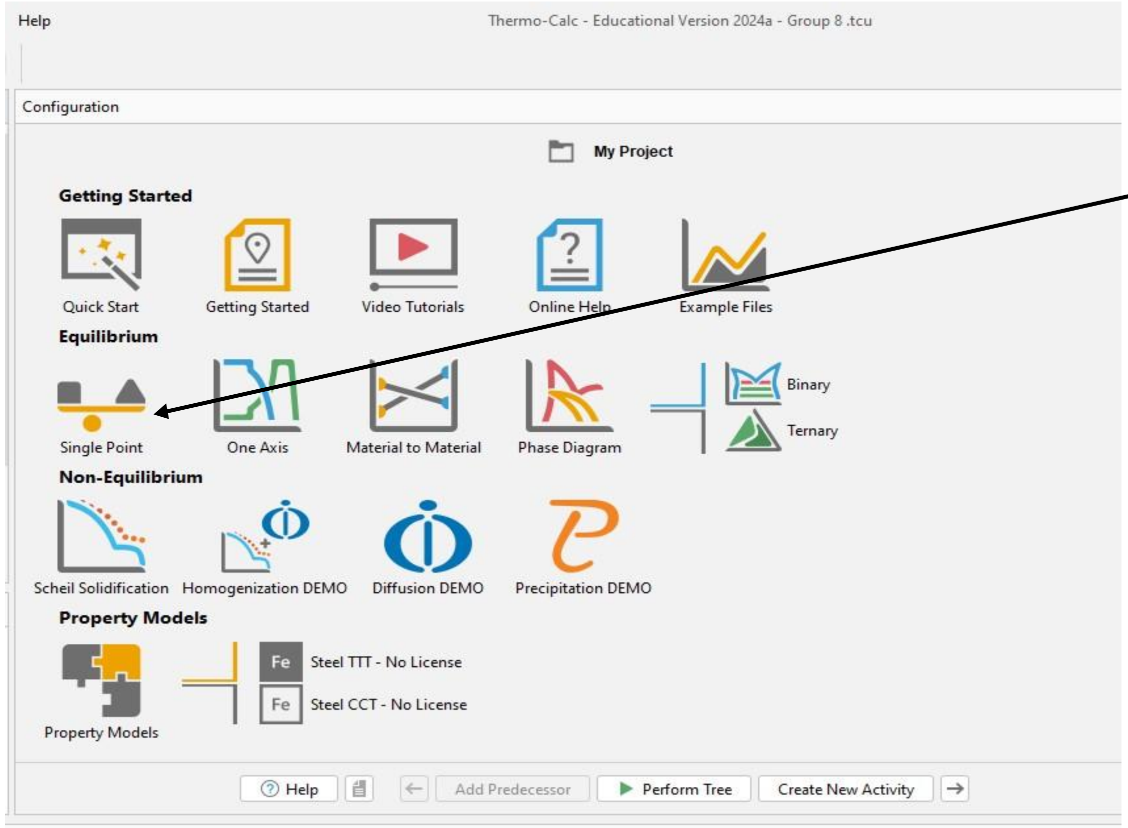
Using DICTRA, simulate the precipitation of Al3Sc particles in the matrix of an Al – 0.3 wt-% Sc alloy. Consider a heat treatment from 650°C to 400°C, with a cooling rate of 5 K/s, followed by isothermal holding.

Width of the region: 2 μm.

Simulation time: 1 hour.
Consider a spherical geometry.

Plot the total phase fraction of Al3Sc and the position of the interface as a function of time.

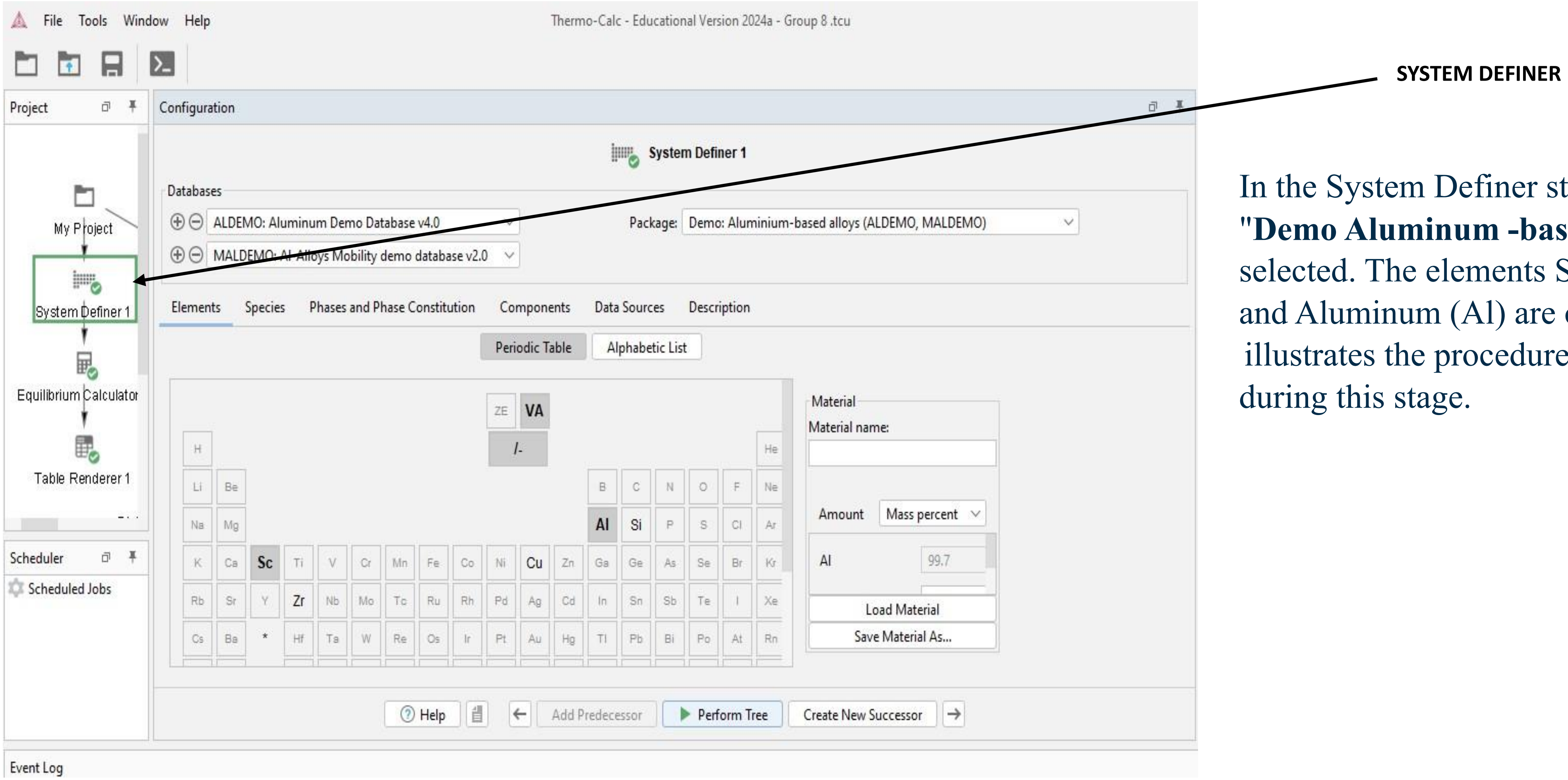
SOLUTION



SINGLE POINT EQUILIBRIUM

Figure 1: A schematic showing the Single Point Equilibrium

Firstly, the phase of the material present at the start of the process needs to be determined. To determine the phase, different approaches can be used by Thermo-Calc In this case, a Single Point Equilibrium calculator used at a temperature of 650°C with a mass percent of 0.3% Scas shown in **Figure 1**.



In the System Definer stage, the package **"Demo Aluminum -based alloys"** was selected. The elements Scandium (Sc) and Aluminum (Al) are chosen. **Figure 2** illustrates the procedures followed during this stage.

Figure 2: A schematic showing the procedures followed in the System Definer.

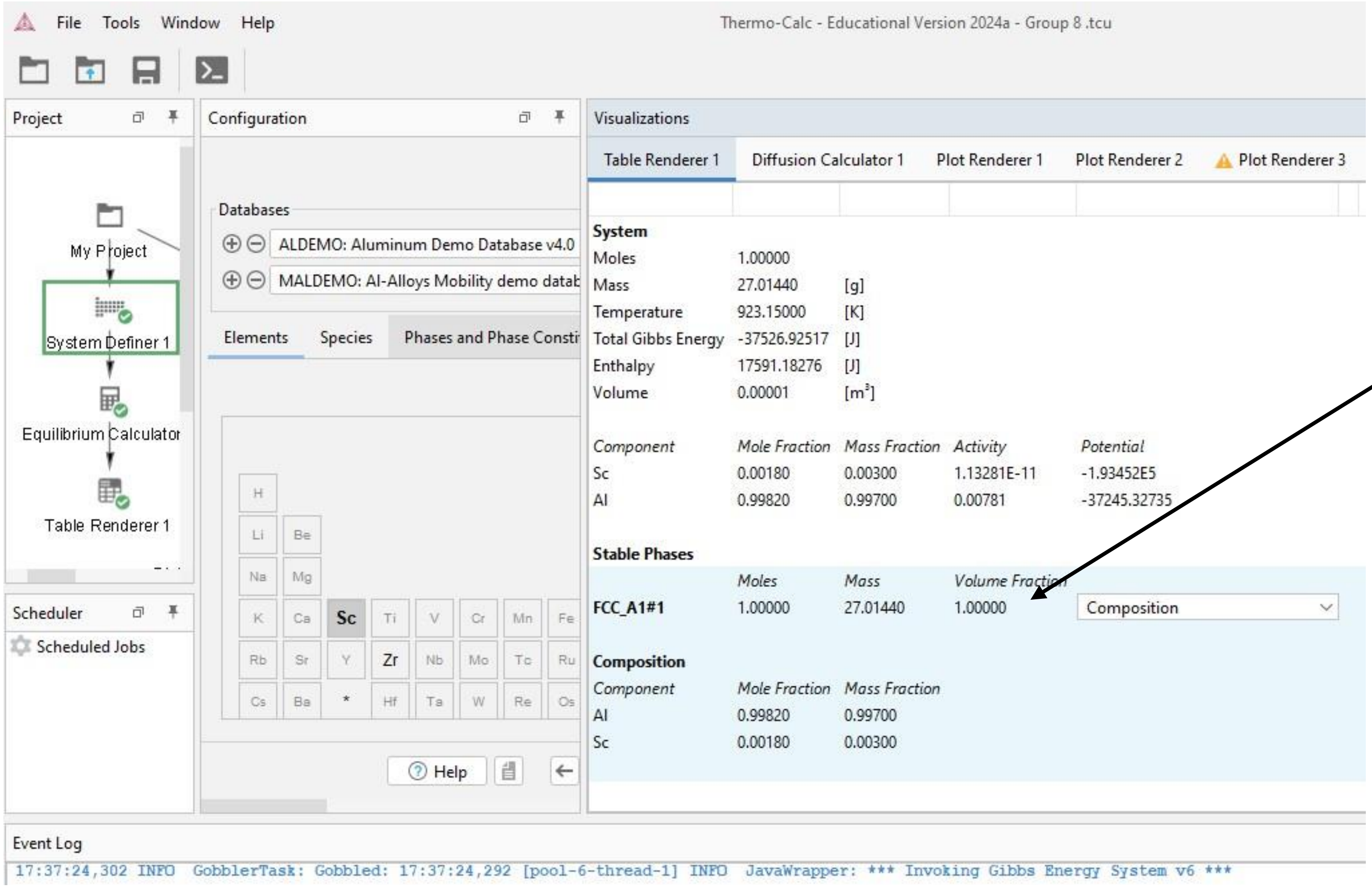


Figure 3 explains **FCC_A1#1** Phase is observed in the composition of Al with Sc at the beginning.

Figure 3: Phase determination at the initial state

- After determining that the phase available in the initial state is FCC_A1#1, a diffusion DEMO simulation was performed to simulate the precipitation of Al_3Sc particles in the matrix of an Al–0.3 wt% Sc alloy.

- The parameters considered for the simulation were predefined as a spherical geometry with a width of 2 micrometers. The aluminum-based alloy package from the database was selected for the simulation.

- The temperature began at 650°C and decreased to 400°C at a rate of 5 Kelvin per second (K/s) for 50 seconds, resulting in a total temperature drop of 250°C. Finally, the system was held isothermally at 400°C for 1 hour.

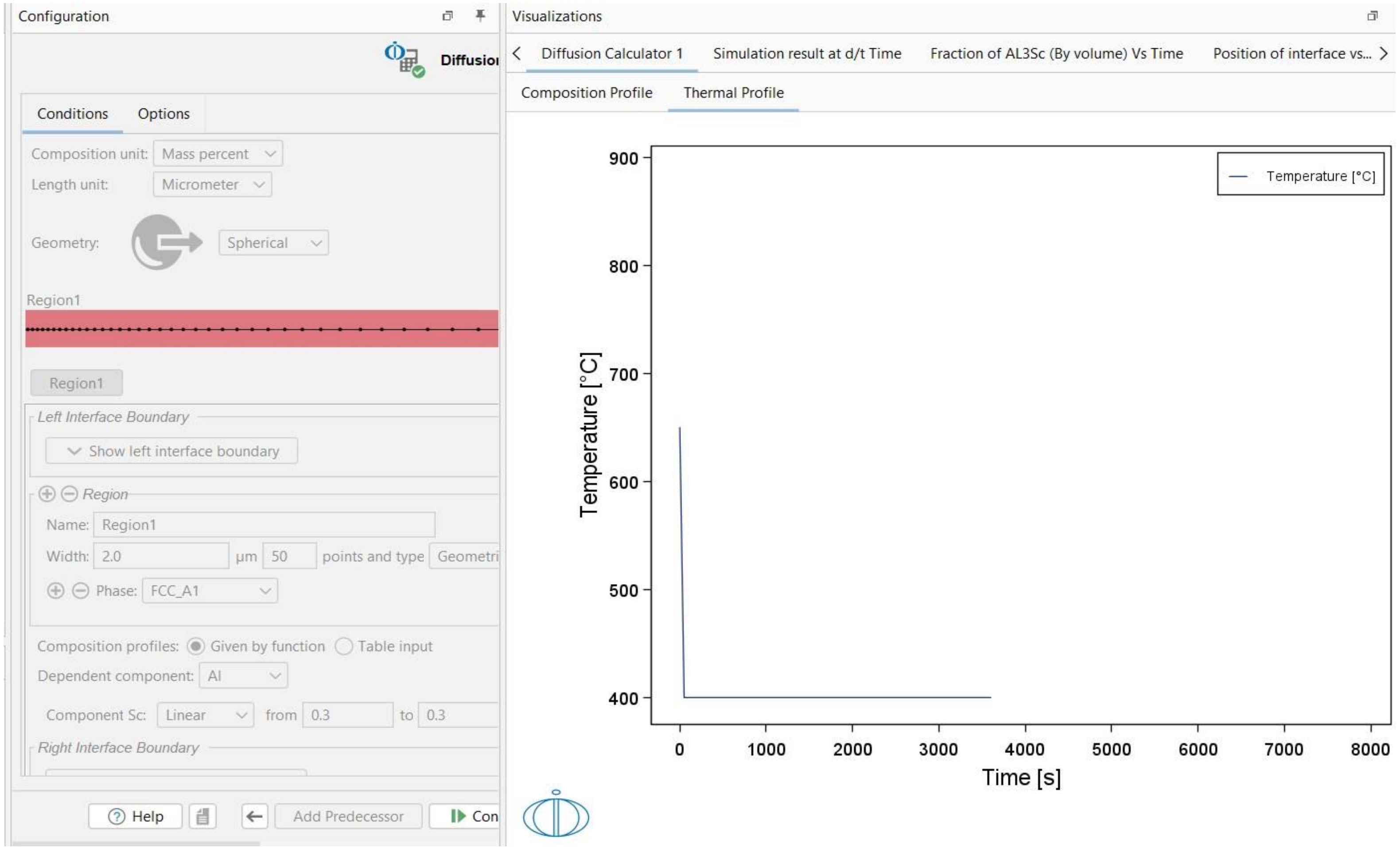


Figure 4: Temperature profile in the process

Figure 4 explains the temperature distribution in the non-isothermal and isothermal cooling under the given time. Also, all simulation parameters such as simulation time mass percent of composition and geometry dimension for **FCC_A1#1** phase are inserted.

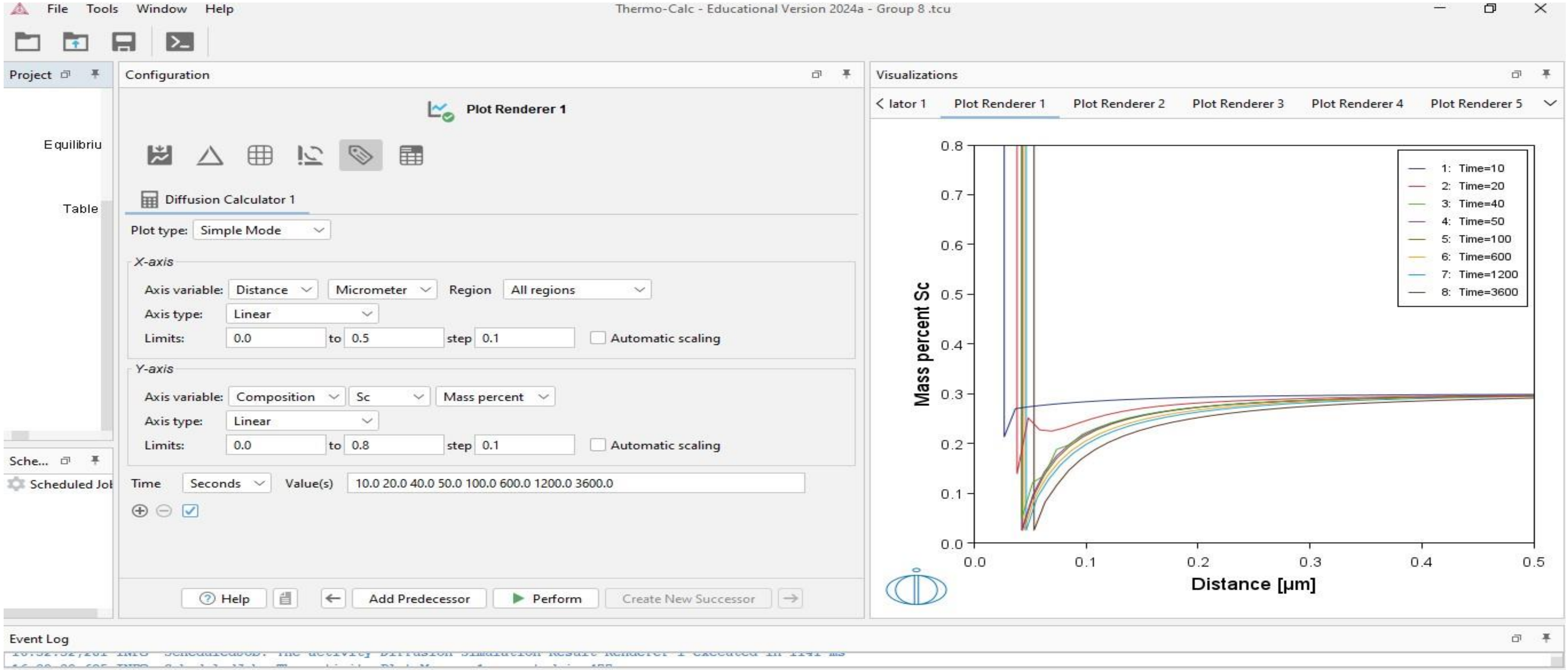


Figure 5: A schematic showing the plot type as Simple Mode, with the X-axis representing distance measured in micrometers with a linear axis type and limits, the Y-axis representing the composition of Sc in mass percent, and time in seconds.

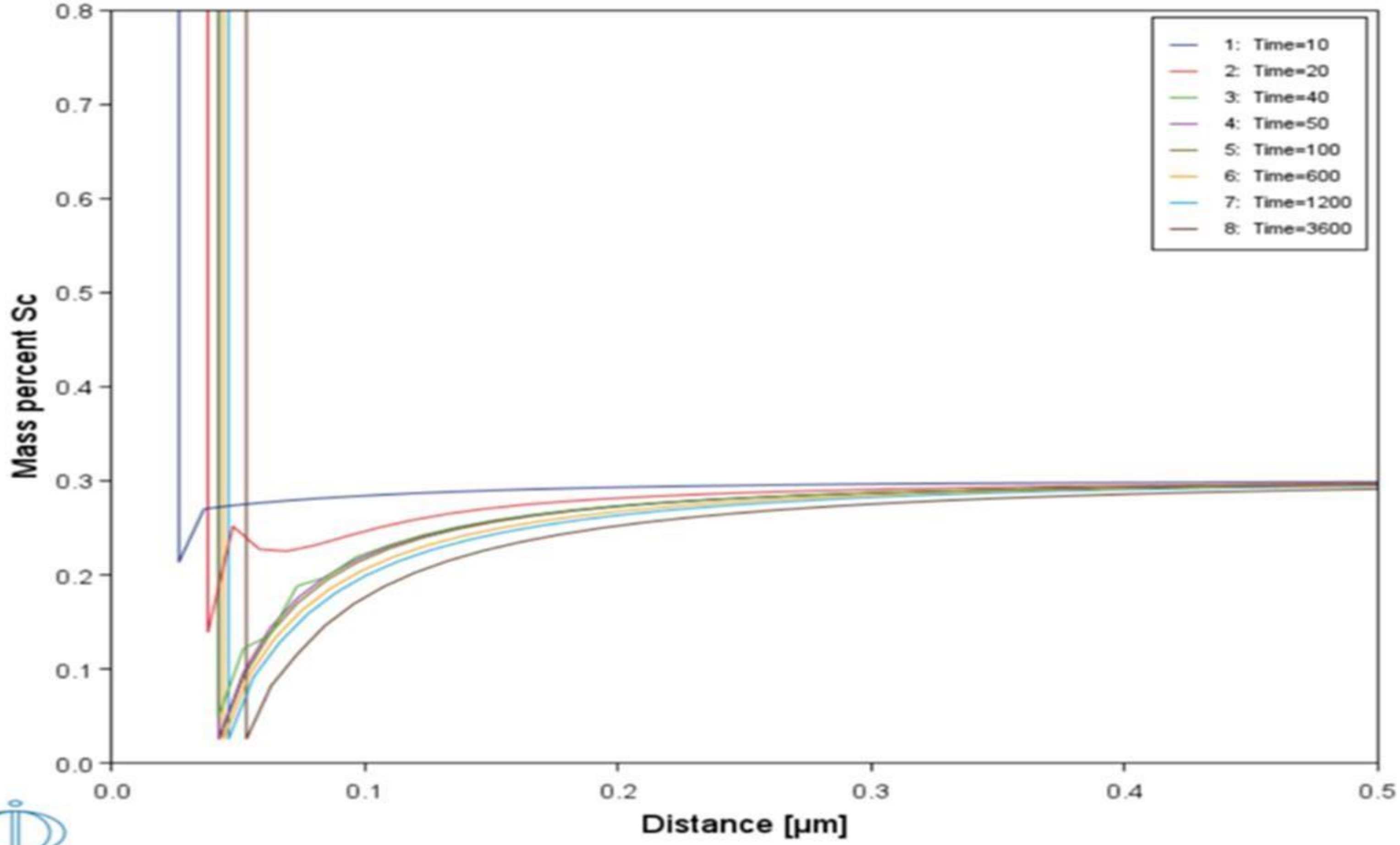


Figure 6: Mass percentage of scandium in the precipitate at different time

The results from the simulation show that the mass percent of Al3Sc particles in the matrix of an Al–0.3 wt% Sc alloy decreases with decreasing temperature. This is because of solid solubility and precipitation at different temperatures, as indicated in **Figure 6**. As the temperature decreases, the solid solubility of Sc in Al decreases. The excess Sc that was previously in solution starts to precipitate as Al3Sc particles. This precipitation process reduces the free Sc available in the matrix, leading to a lower mass percent of Al3Sc particles.

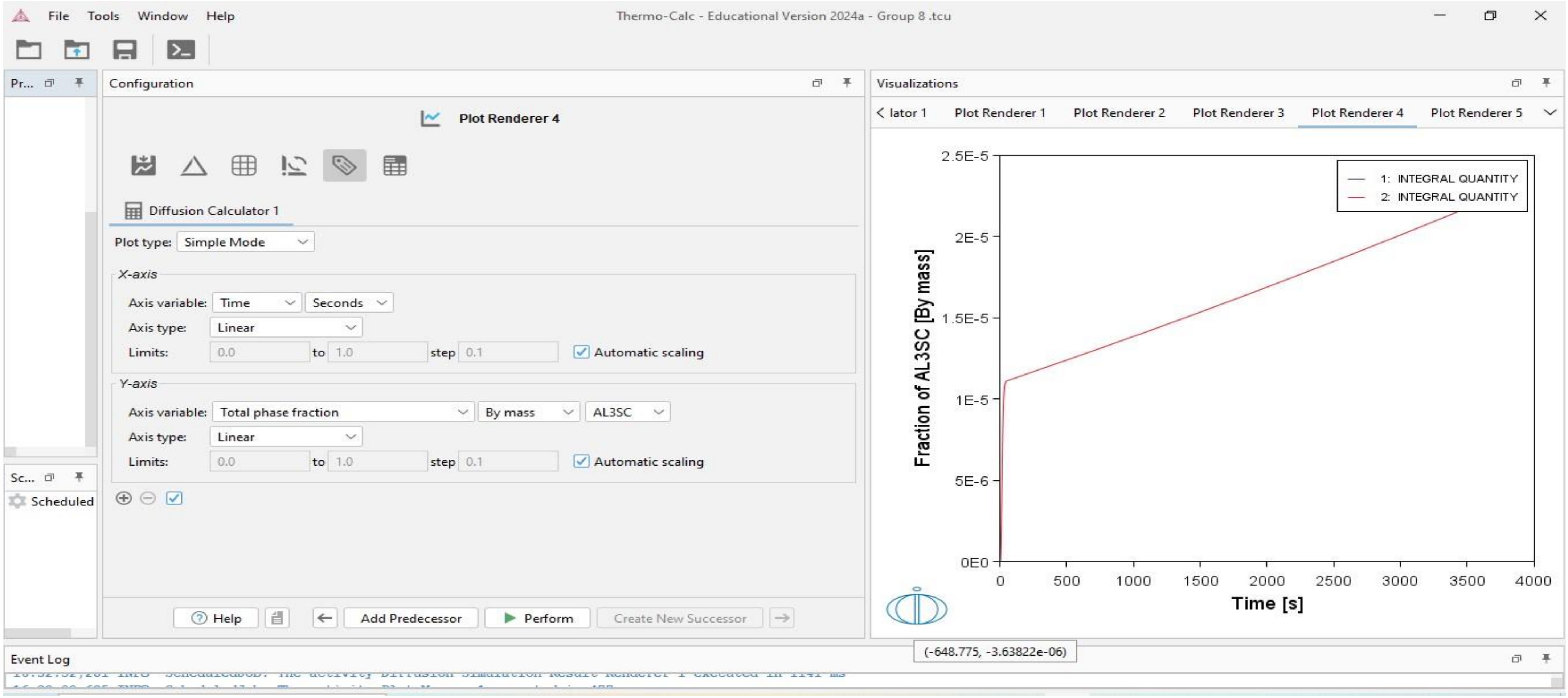


Figure 7: A schematic showing the plot type as Simple Mode, with the X-axis representing time measured in seconds (axis type Linear) and the Y-axis representing the total phase fraction by mass of Al3Sc (axis type Linear).

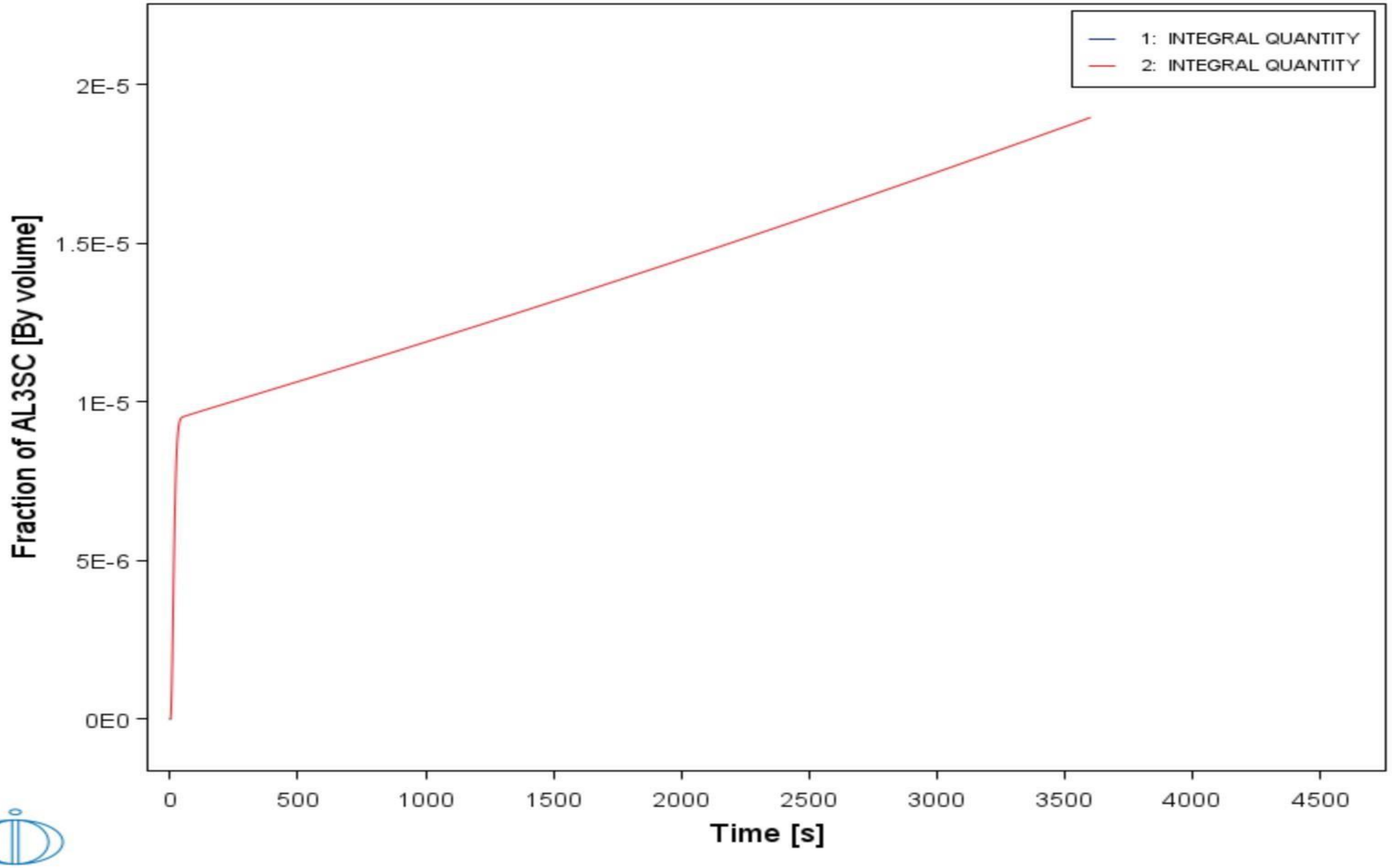


Figure 8: Total phase fraction of AL3SC vs Time

Figure 8 shows the volume fraction of Al3Sc in the particle at the start of the process. In this phase, where both FCC_A1#1 and Al3Sc are stable, there is an immediate increase in the fraction of Al3Sc. This increase results from the introduction of predefined Al3Sc particles into the model. Subsequently, through diffusion, the fraction continues to grow.

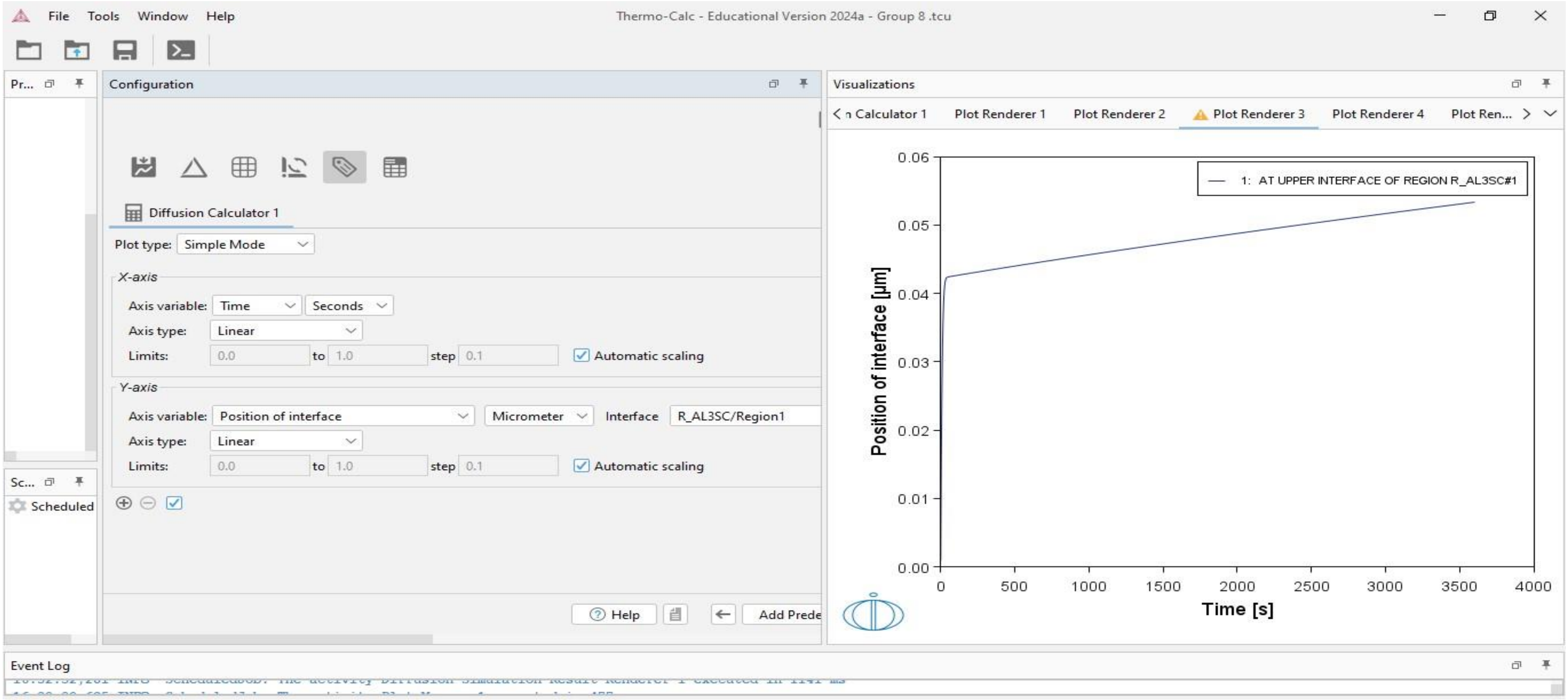


Figure 9: A schematic with the plot type set as Simple Mode. The X-axis represents time measured in seconds, with a linear axis type. The Y-axis represents the position of the interface in micrometers, denoted as R_AL3SC/Region1, also with a linear axis type.

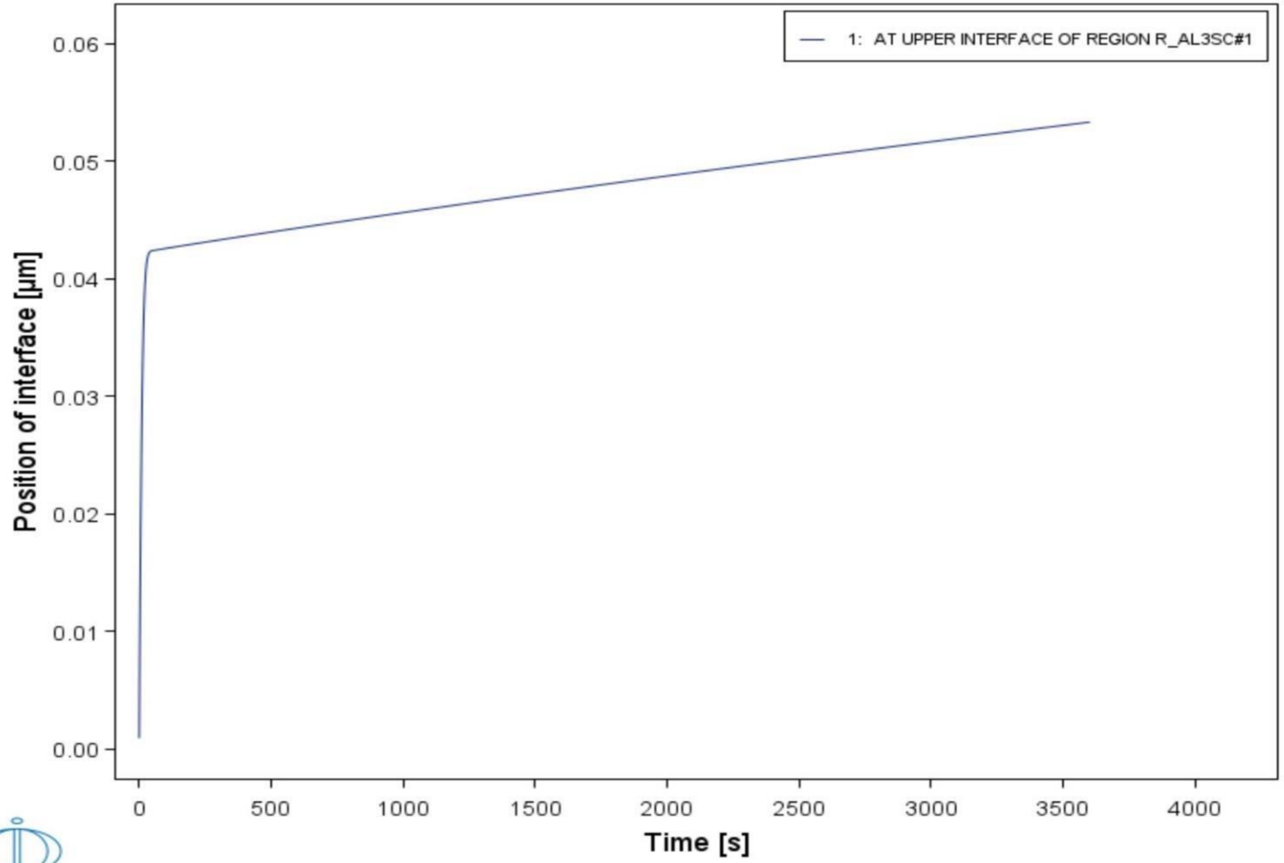


Figure 10: Position interface vs Time

Figure 10 shows an initial rapid rise in interface position from 0 to about 0.020 µm at the start, which then gradually increases to roughly 0.042 µm. Afterwards, the graph shows time advancing swiftly past 50 seconds and then to 3600 seconds, with only a slight increase in interface position. This indicates an initial phase of fast nucleation and growth, followed by a significantly slower growth phase, likely controlled by diffusion processes as the system stabilizes during the extended isothermal holding at 400°C.

END

Politecnico di Torino
1859

MATERIALS AND DESIGN

THERMO-CALC REPORT 2

Politecnico di Torino

1859

NAMES	STUDENT ID
Siriro, Wiseman	S333263

POLYTECHNIC UNIVERSITY OF TURIN

ITALY

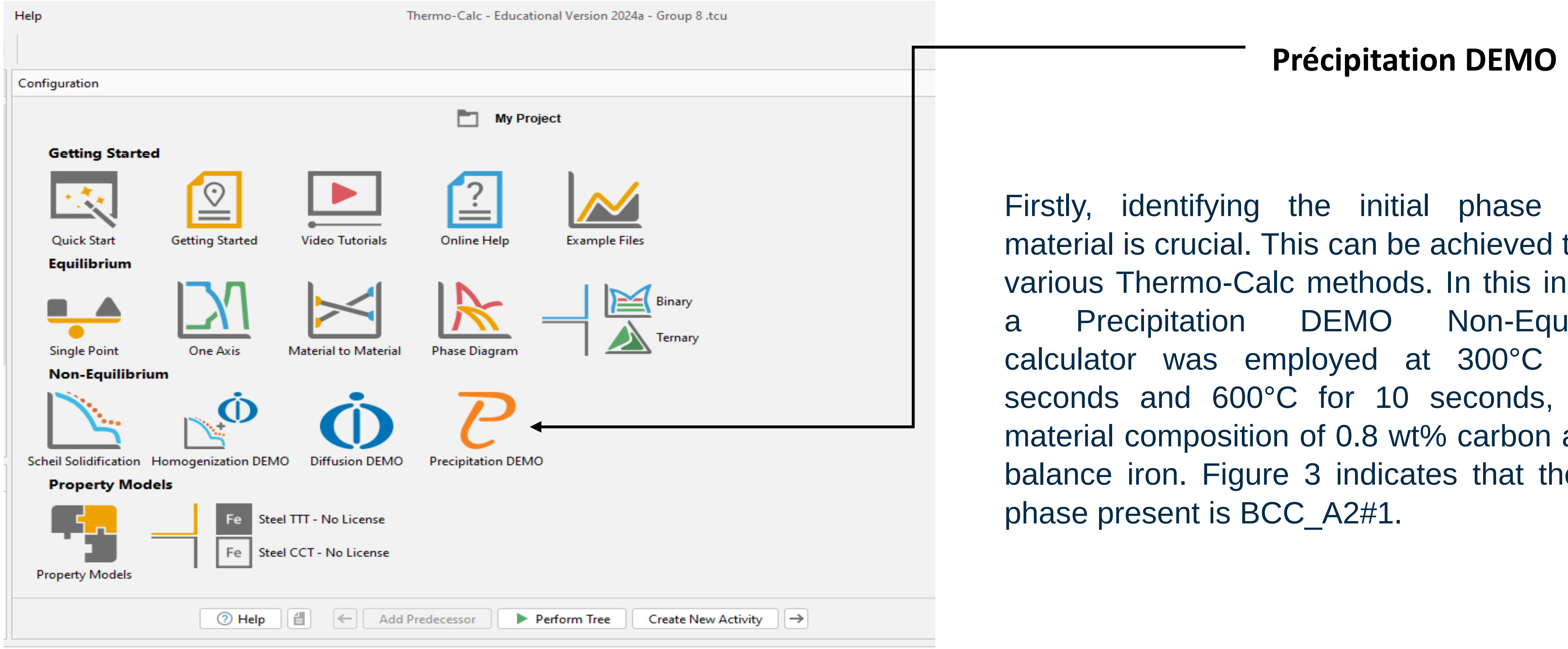
QUESTION

Simulate the kinetics of precipitation of cementite in steel in two different cases.
First, consider isothermal precipitation at 300°C for 10 s.
Then, perform a new simulation, considering isothermal precipitation at 600°C for 10 s.

Material: C: 0.8 wt%; Fe: balance
For the two heat treatments, compute:
- The average precipitate size as a function of time
- The nucleation rate as a function of time
- The number density of cementite as a function of time
- The trend of yield strength as a function of time.

In the two cases, how are the nucleation rate, the average precipitate size, and the mechanical properties correlated? Briefly comment on this (max 300 words).
How does the temperature influence the precipitation process?

SOLUTION



Firstly, identifying the initial phase of the material is crucial. This can be achieved through various Thermo-Calc methods. In this instance, a Precipitation DEMO Non-Equilibrium calculator was employed at 300°C for 10 seconds and 600°C for 10 seconds, with a material composition of 0.8 wt% carbon and the balance iron. Figure 3 indicates that the initial phase present is BCC_A2#1.

Figure 1: A schematic showing various modules and tools available for equilibrium and non-equilibrium thermodynamic calculations, property models, and educational resources.

SYSTEM DEFINER

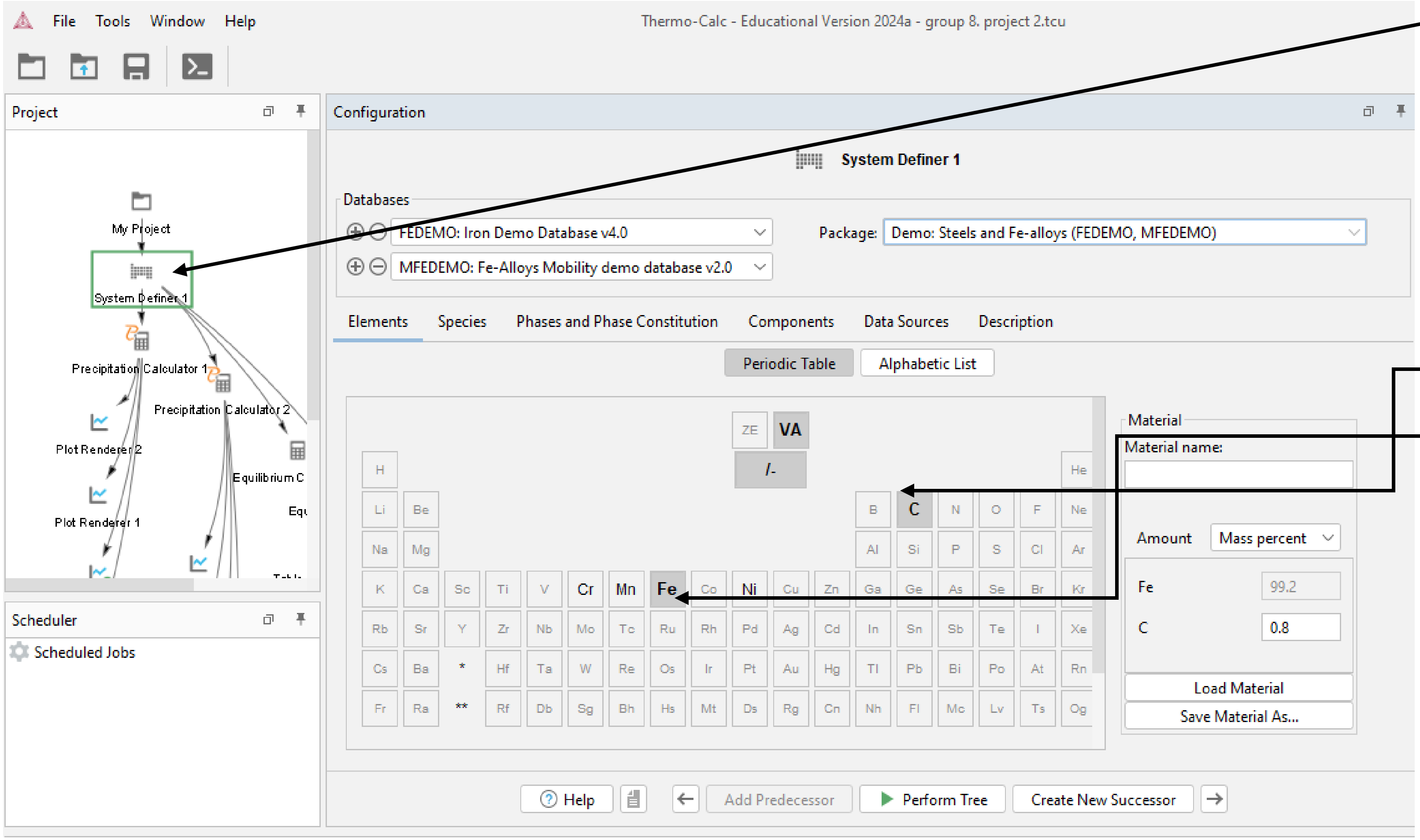


Figure 2: A schematic showing the procedures followed in the System Definer.

In the System Definer stage, the package " Demo: Steels and Fe alloys" was selected. The elements carbon (C) and iron (Fe) were chosen. Figure 2 illustrates the procedures followed during this stage.

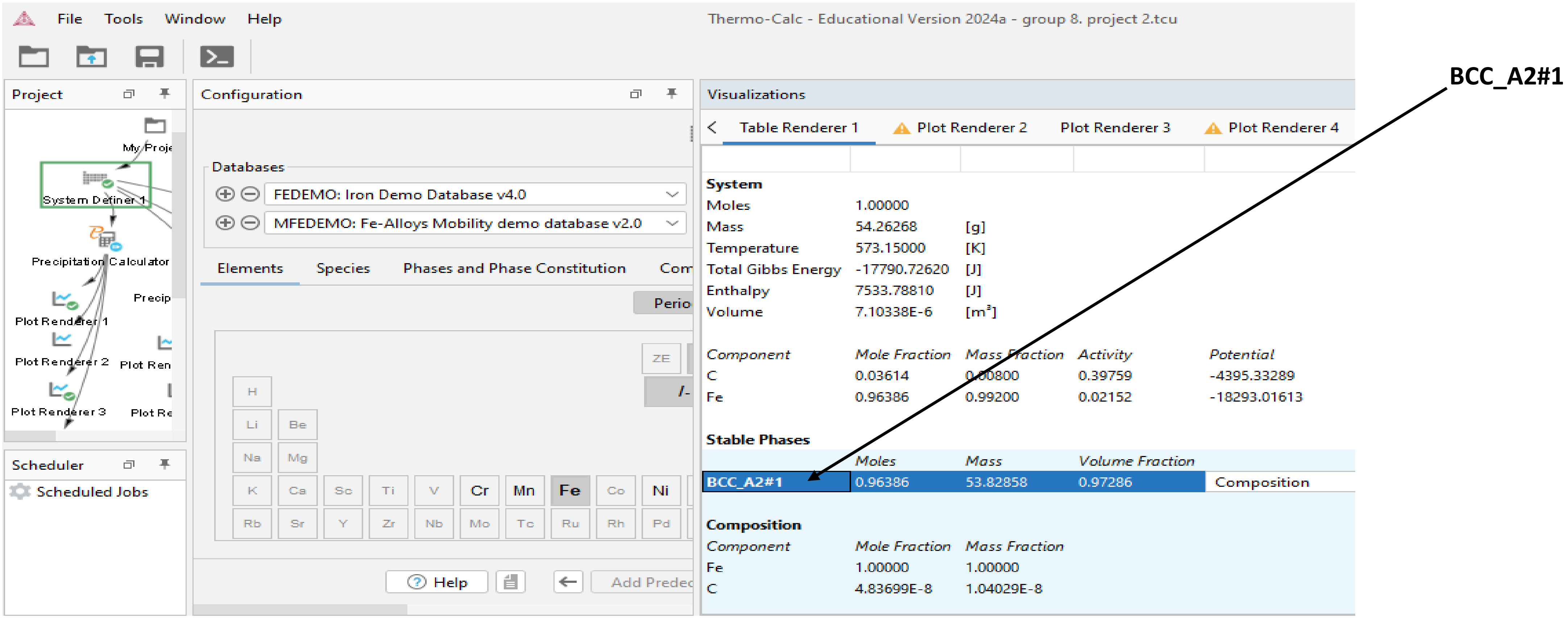


Figure 3. Phase determination at the initial state

- After determining that the phase available in the initial state is BCC_A2#1, a Précipitation DEMO simulation was performed to Simulate the kinetics of precipitation of cementite in steel in two different cases.

- Firstly, a simulation considering isothermal precipitation at 300°C for 10 seconds was performed. The material composition was 0.8 wt% carbon, with the balance being iron. For this heat treatment, the following parameters were computed: the average precipitate size as a function of time, the nucleation rate as a function of time, the number density of cementite as a function of time, and the trend of yield strength as a function of time.

- Secondly, a simulation was conducted to study isothermal precipitation at 600°C for 10 seconds. The material composition was 0.8 wt% carbon, with the remainder being iron. During this heat treatment, the following were computed: the average precipitate size over time, the nucleation rate over time, the number density of cementite over time, and the trend of yield strength over time.

SIMULATION CONSIDERING ISOTHERMAL PRECIPITATION AT 300°C FOR 10 S.

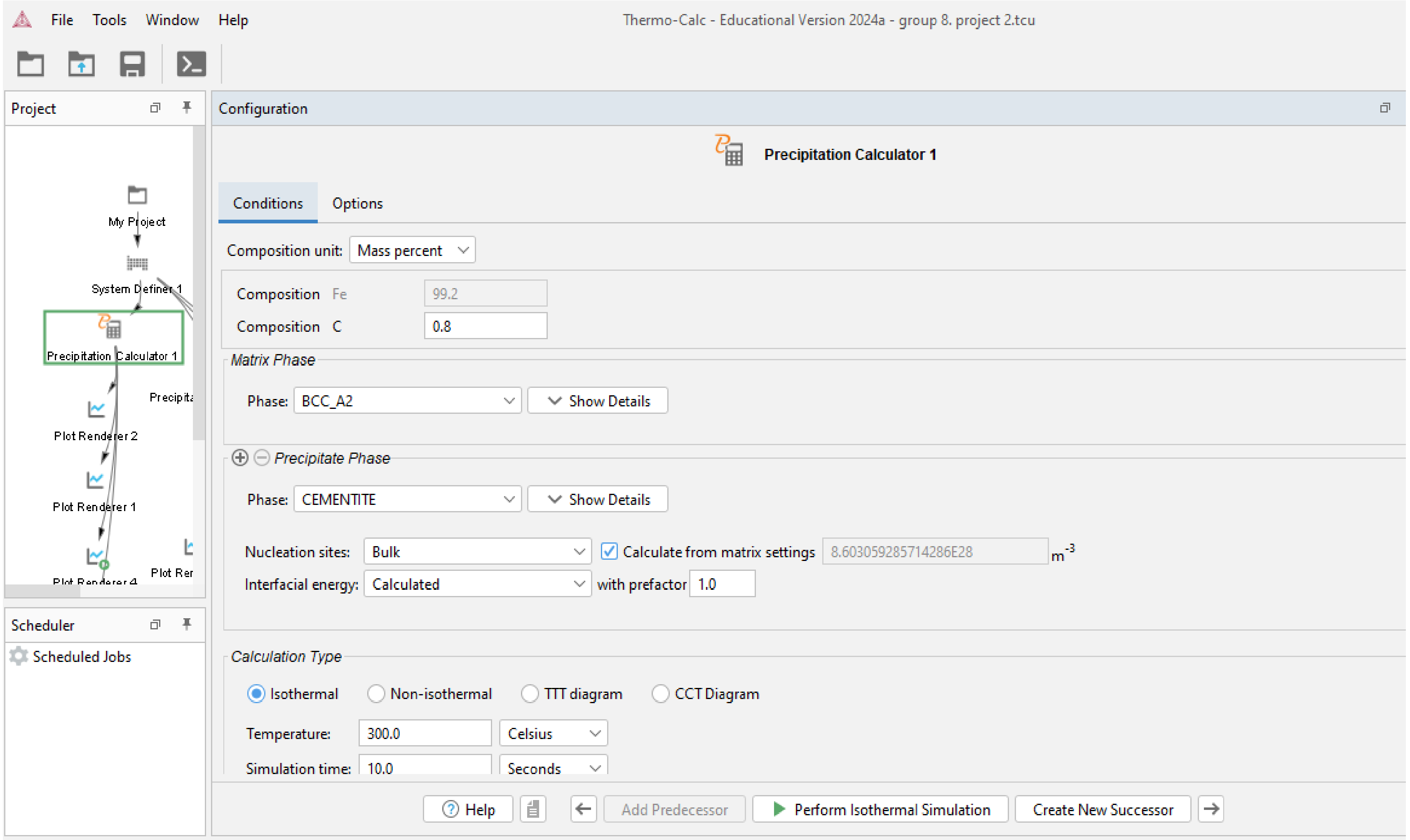


Figure 4: The precipitation calculation where isothermal precipitation was considered to be at 300°C for 10 seconds

Figure 4 shows the precipitation calculation where isothermal precipitation was considered to be at 300°C, while the simulation time was set to 10 seconds. The composition of C was 0.8 mass percent, and BCC_A2 was the matrix phase. Figure 5 shows an isothermal precipitation simulation at 300°C for 10 seconds, confirming a constant temperature throughout the duration. This simulation provides an understanding of how cementite precipitates form and evolve under these specific conditions (300°C for 10 seconds).

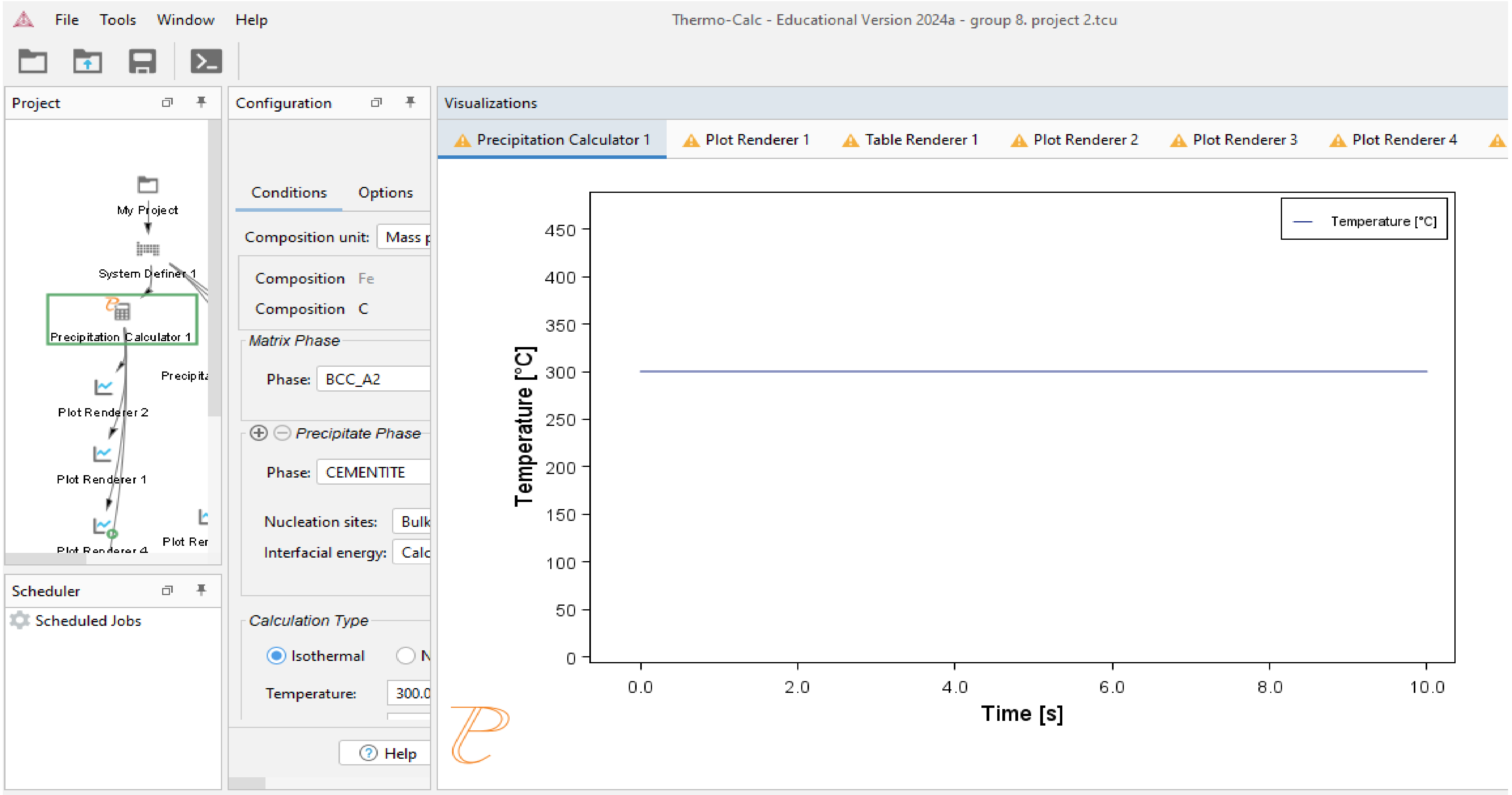


Figure 5. Temperature profile in the process

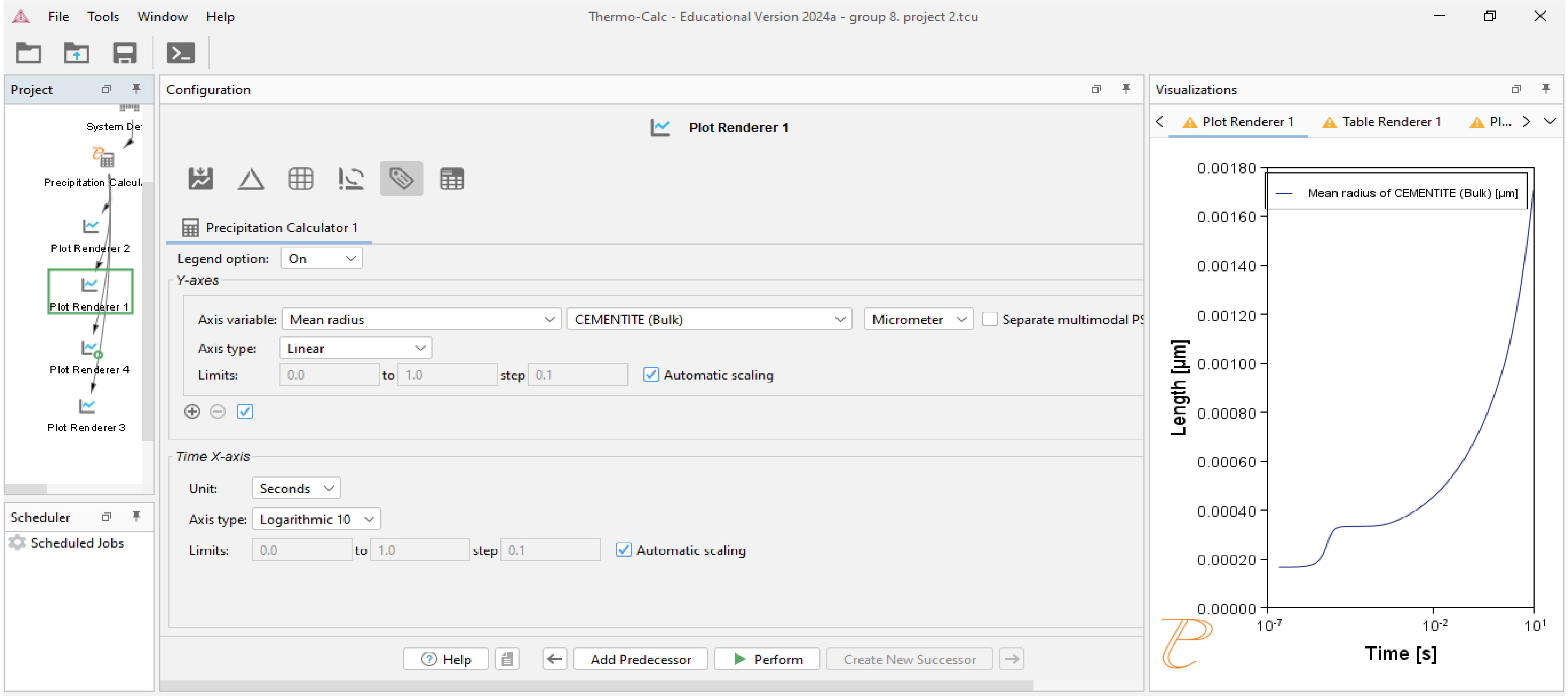


Figure 6: A schematic showing the legend option, with the X-axis representing time measured in seconds with a logarithm base 10 axis type and limits, and the Y-axis representing the mean radius of Cementite (Bulk) in micrometers with a linear axis type.

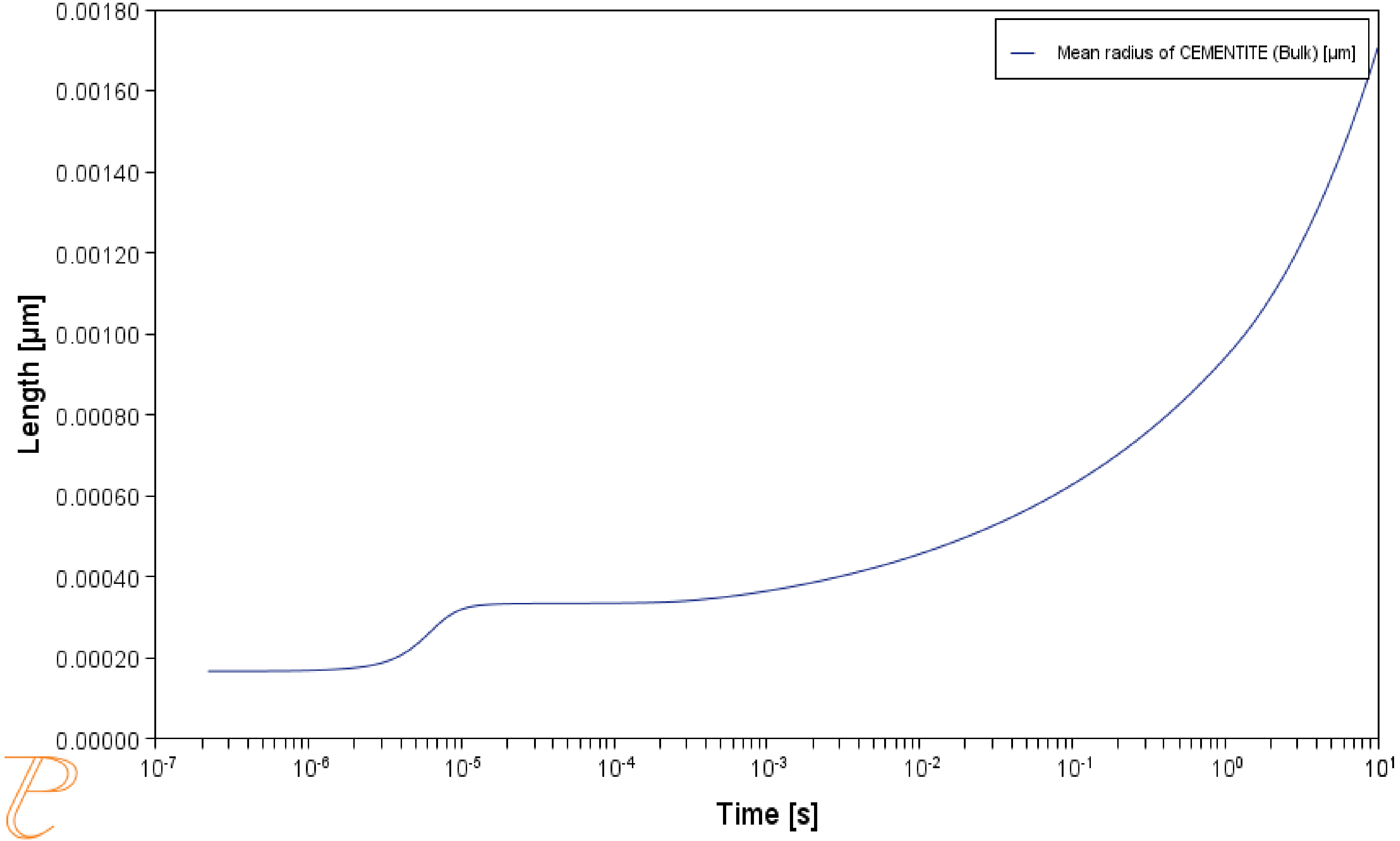


Figure 7. Mean radius of Cementite (Bulk) in the precipitate

The diagram shows the mean radius of bulk cementite precipitates as a function of time on a logarithmic scale. Initially, there is a very slow increase in the mean radius of cementite, indicated by a nearly flat line, suggesting a lag phase where nucleation and initial growth are minimal. As time progresses, a slight inflection point is observed, indicating the onset of more significant growth. After this inflection, the growth rate of the mean radius of cementite increases rapidly, particularly after 0.0001 seconds, with a sharp rise evident approaching 10 seconds. This pattern indicates that, following an initial slow nucleation and growth phase, cementite particles experience accelerated growth, likely driven by increased diffusion and coarsening processes at the given temperature.

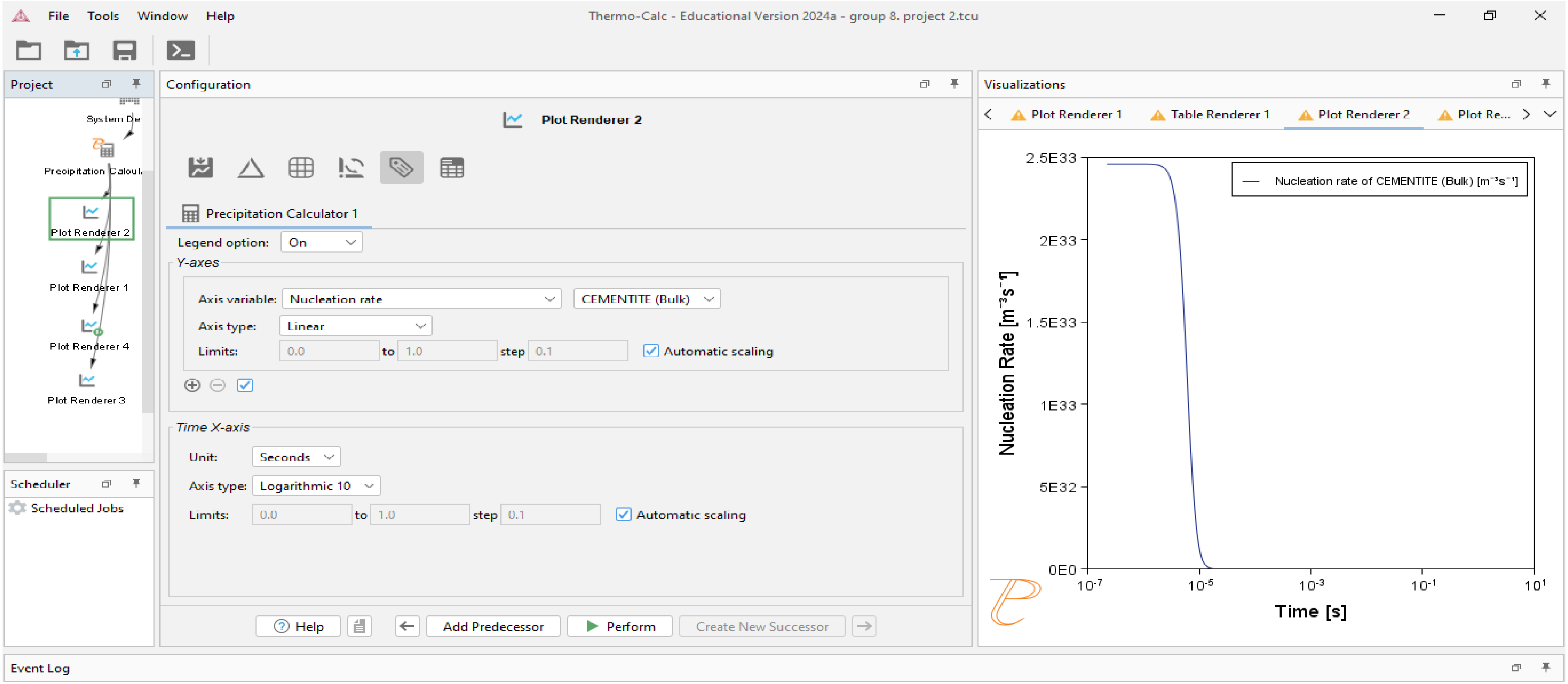


Figure 8: A schematic showing the legend option, with the X-axis representing time measured in seconds with a logarithm base 10 axis type and limits, and the Y-axis representing the nucleation rate of Cementite (Bulk) with a linear axis type.

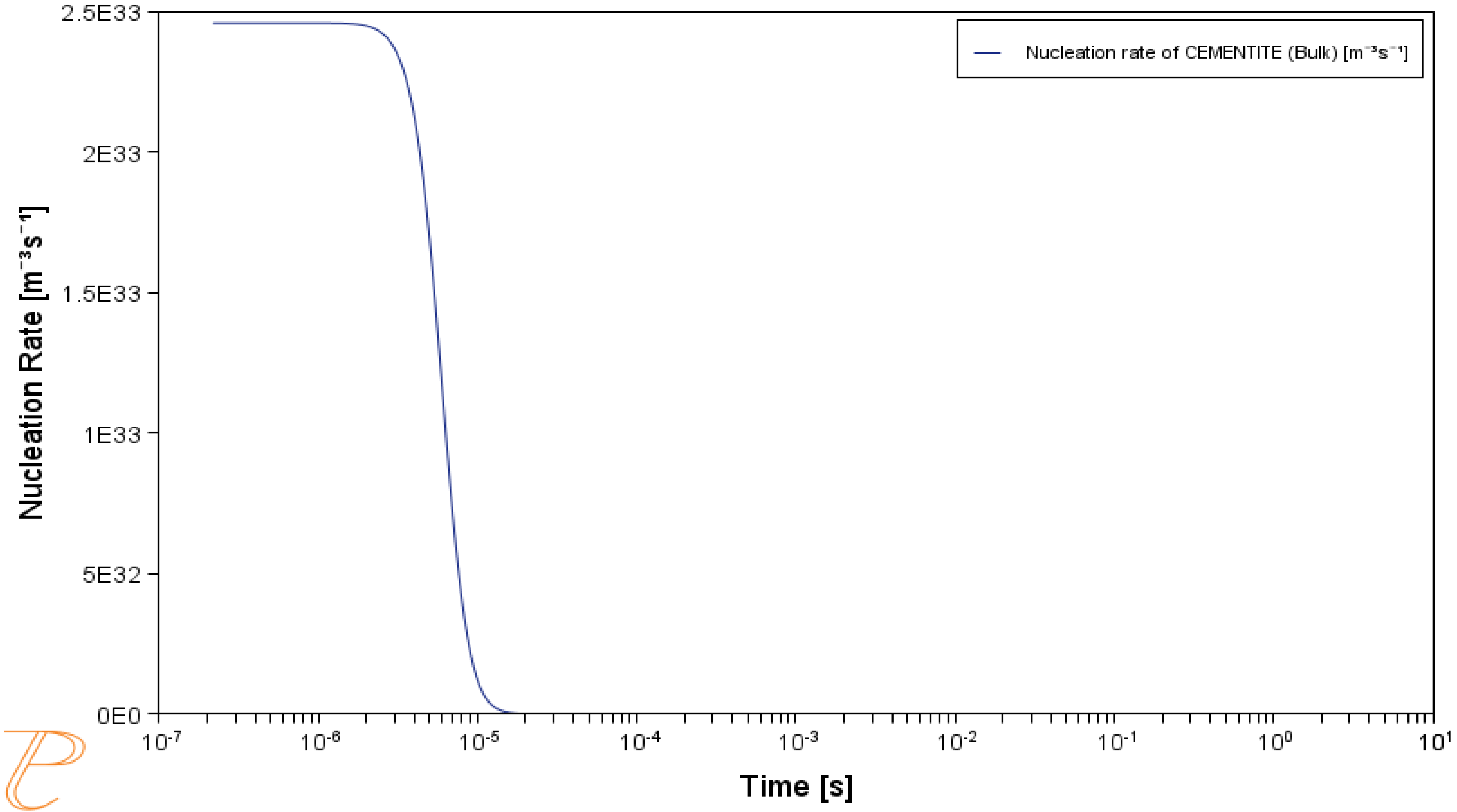


Figure 9. The Nucleation rate as a function of Time

The graph shows the nucleation rate of cementite in bulk as a function of time on a logarithmic scale. Initially, the nucleation rate is extremely high, indicating rapid formation of nuclei due to favorable conditions such as high supersaturation. Around 0.00001 seconds, the rate sharply decreases, suggesting a depletion of nucleation resources or a shift in conditions making nucleation less favorable. Eventually, the rate levels off to nearly zero, indicating that nucleation has largely ceased, likely due to reaching a stable state where further nucleation is rare.

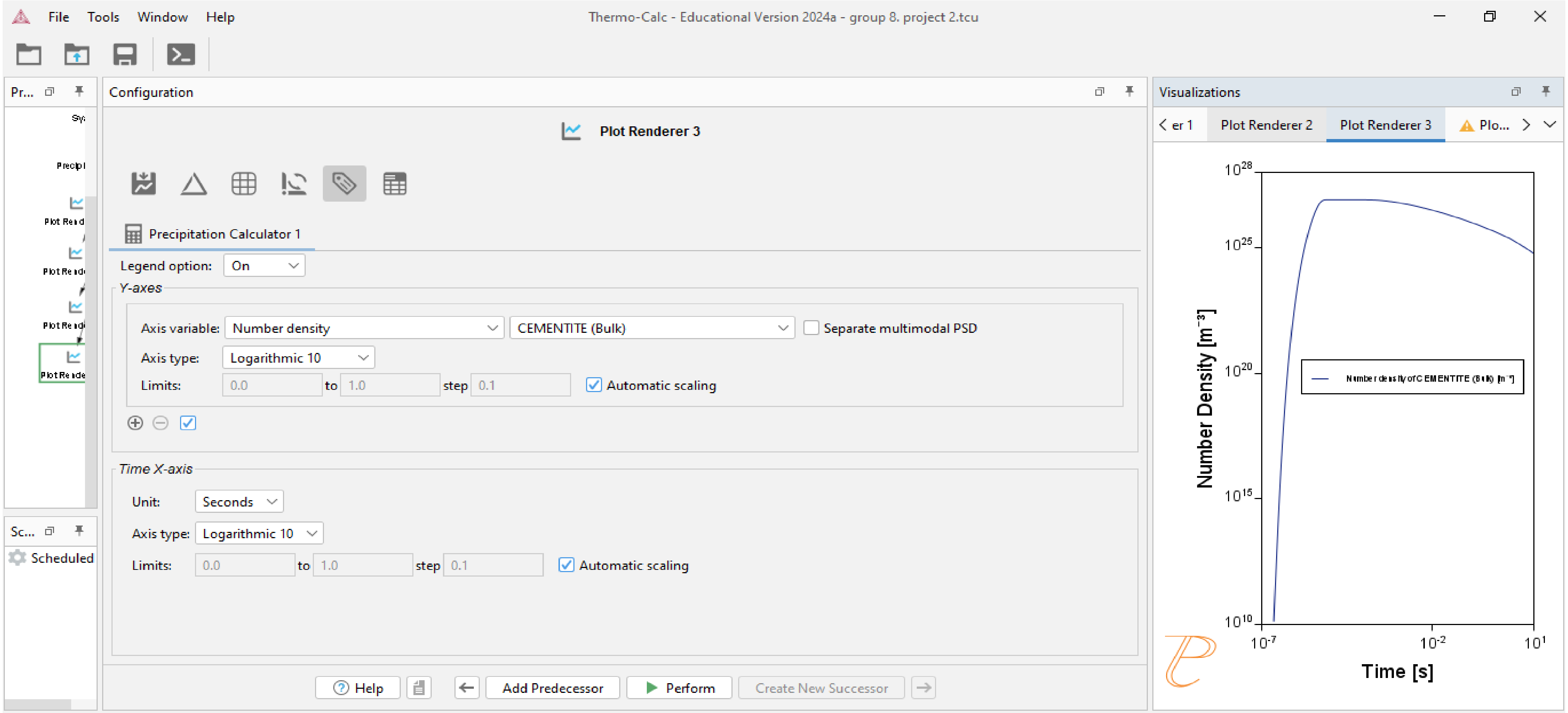


Figure 10: A schematic showing the legend option, with the X-axis representing time measured in seconds using a logarithmic base 10 scale, and the Y-axis representing the number density of cementite (bulk) using a logarithmic base 10 scale.

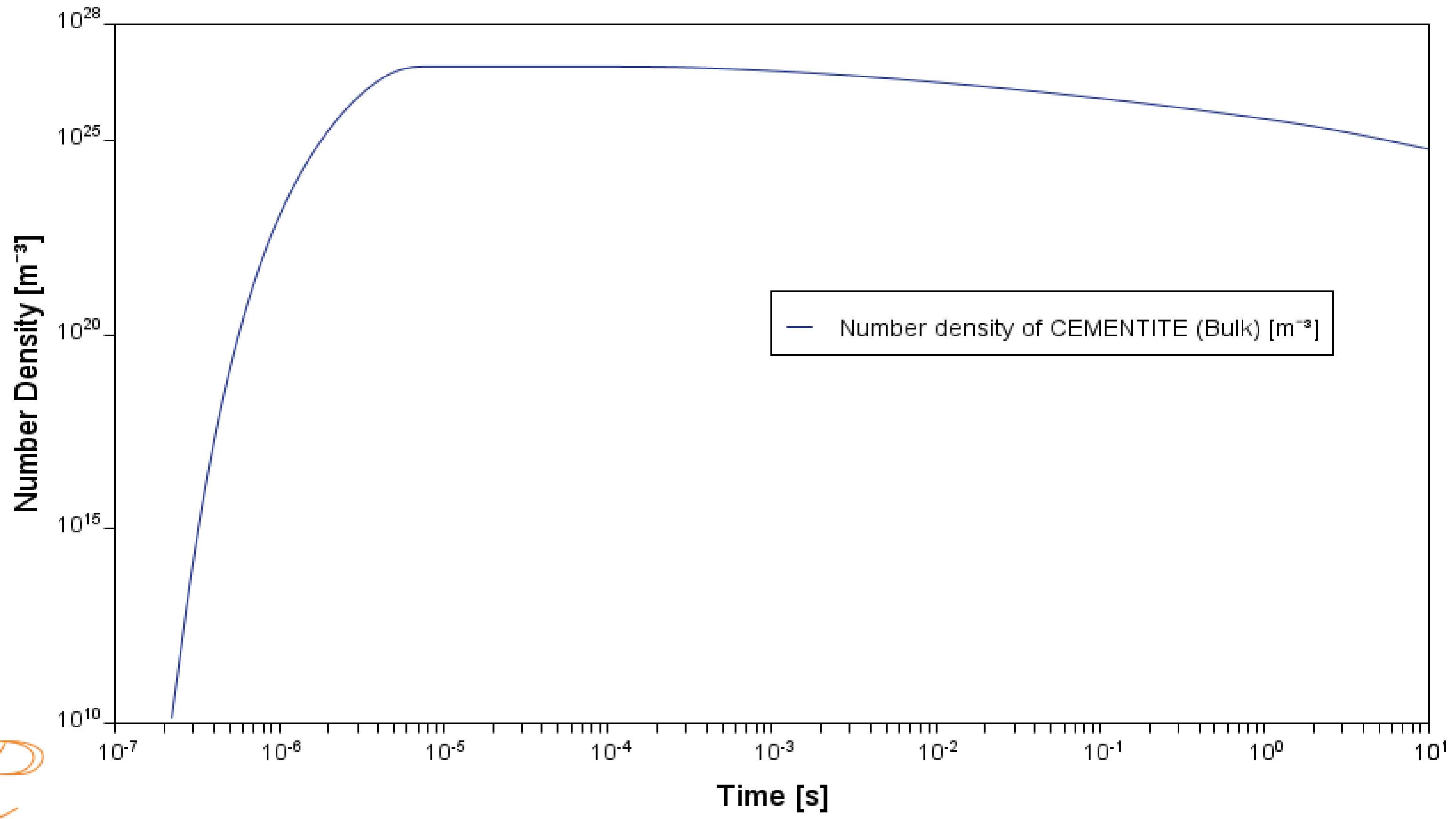


Figure 11. The number density of cementite as a function of time

Figure 11. shows the number density of cementite in bulk material as a function of time. Initially, there is a rapid increase in number density, peaking around 0.00001 seconds, indicating rapid nucleation and formation of cementite particles. Following the peak, the number density gradually declines, likely due to processes where larger particles grow at the expense of smaller ones, phase transformations, or dissolution, reducing the number of cementite particles over time. The graph illustrates the dynamic formation and stabilization behavior of cementite in the material.

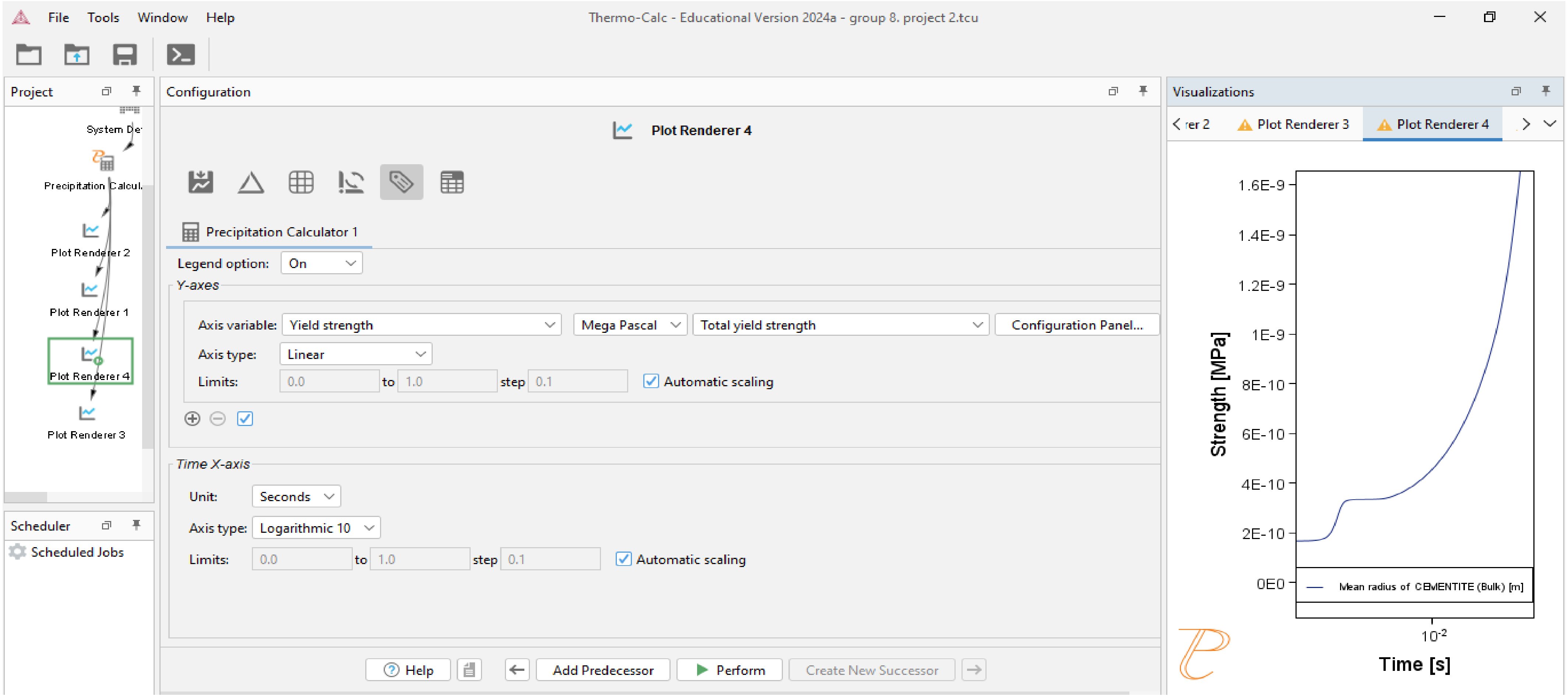


Figure 12: A schematic showing the legend option, with the X-axis representing time measured in seconds with a logarithm base 10 axis type and limits, and the Y-axis representing the yield strength of Cementite (Bulk) in megapascals with a linear axis type.

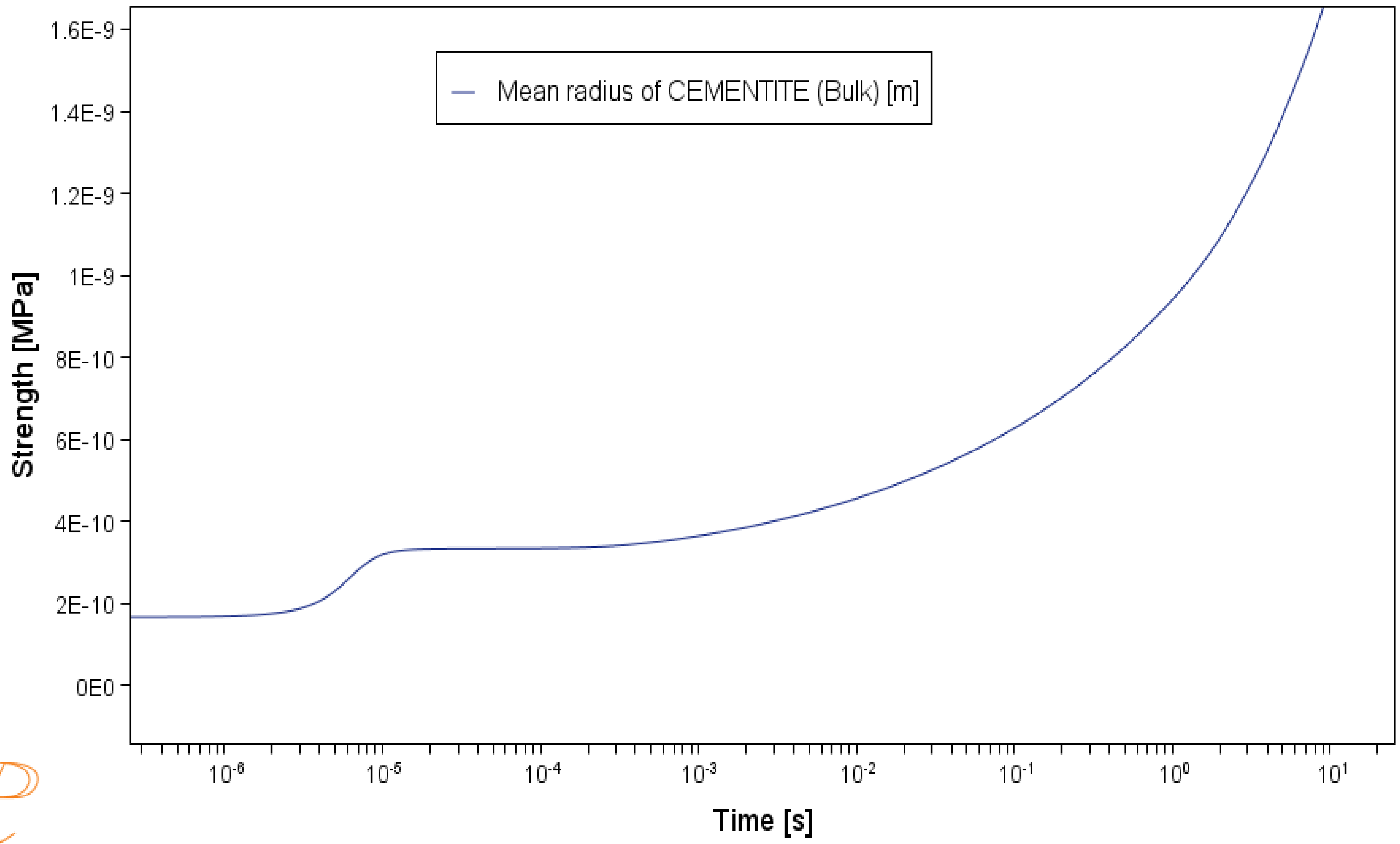


Figure 13. The trend of yield strength as a function of time.

The diagram shows the trend of yield strength as a function of time, focusing on the mean radius of cementite in bulk material. Initially, for very short times (less than 0.00001 seconds), the yield strength is very low and remains almost constant. Around 0.00001 to 0.0001 seconds, there is a slight increase in yield strength. As time progresses further, especially beyond 0.001 seconds, the yield strength begins to increase more rapidly, following an upward curve. This trend suggests that the yield strength of the material increases as the mean radius of cementite particles grows over time, likely due to the hardening effects caused by the formation and coarsening of cementite within the material's microstructure.

Simulation considering isothermal precipitation at 600°C for 10 s

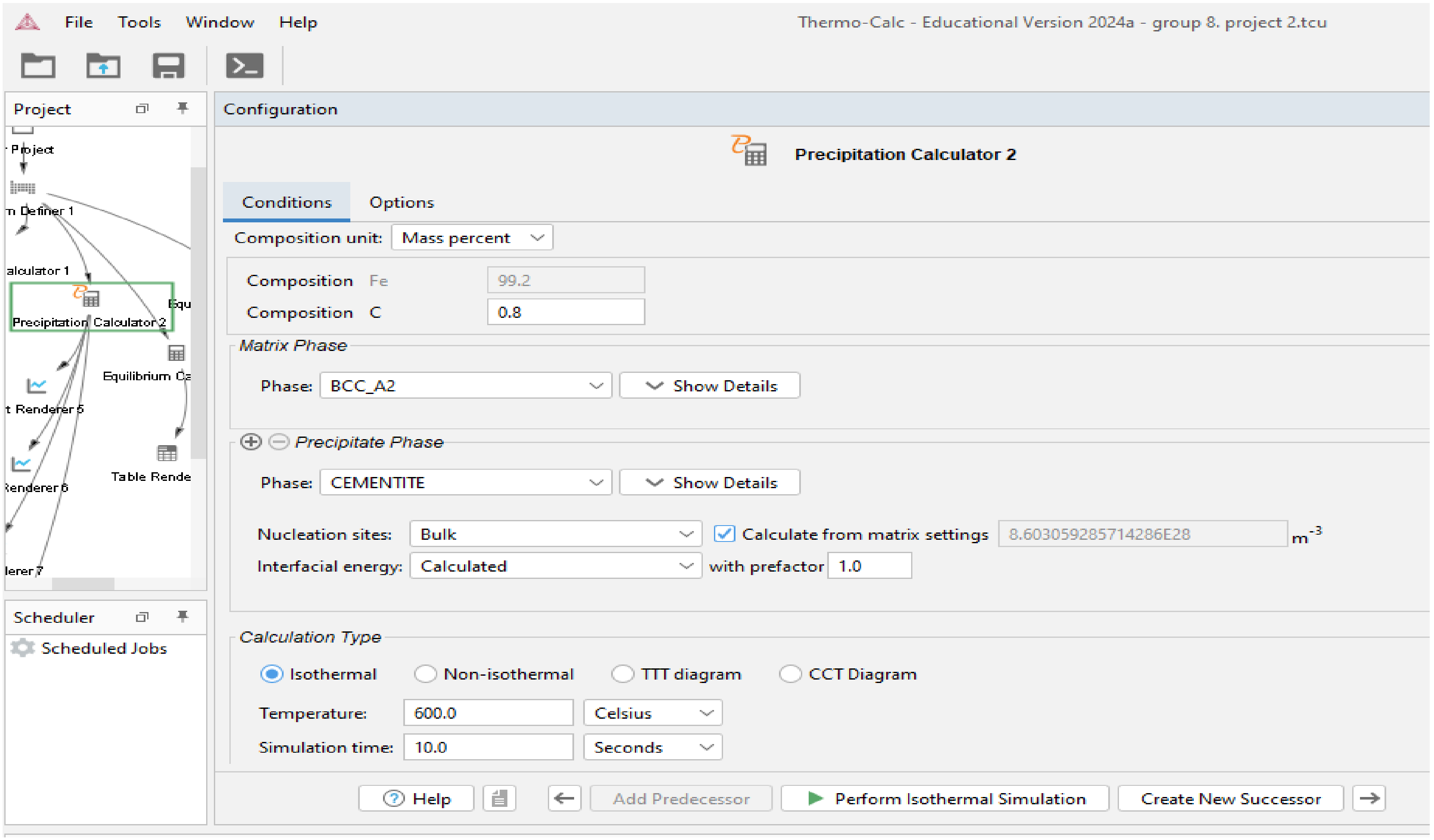


Figure 14: The precipitation calculation where isothermal precipitation was considered to be at 600°C for 10 seconds

Figure 14 shows the precipitation calculation where isothermal precipitation was considered to be at 600°C, while the simulation time was set to 10 seconds. The composition of C was 0.8 mass percent, and BCC_A2 was the matrix phase. Figure 15 shows an isothermal precipitation simulation at 600°C for 10 seconds, confirming a constant temperature throughout the duration. This simulation provides an understanding of how cementite precipitates form and evolve under these specific conditions (600°C for 10

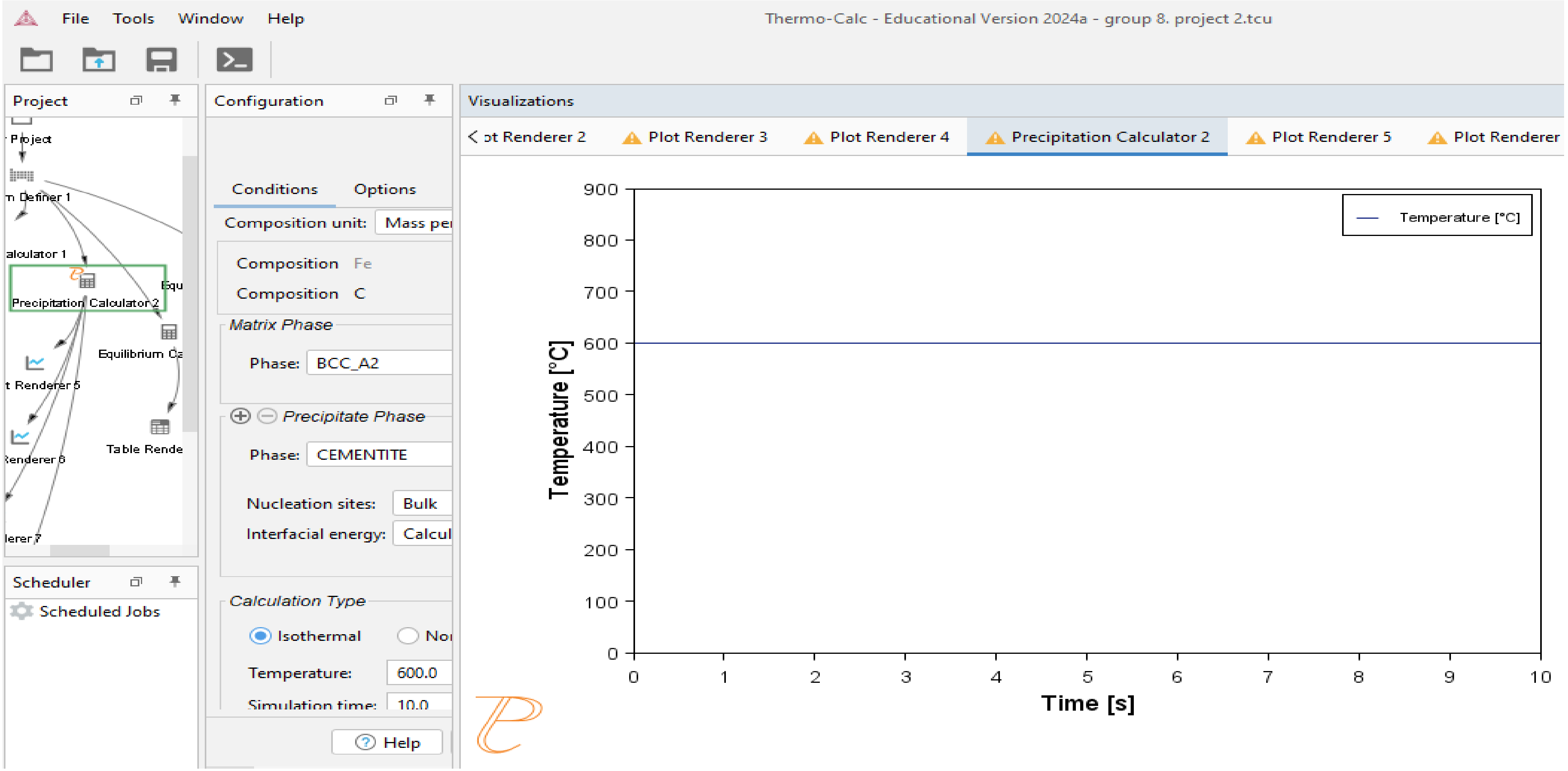


Figure 15. Temperature profile in the process

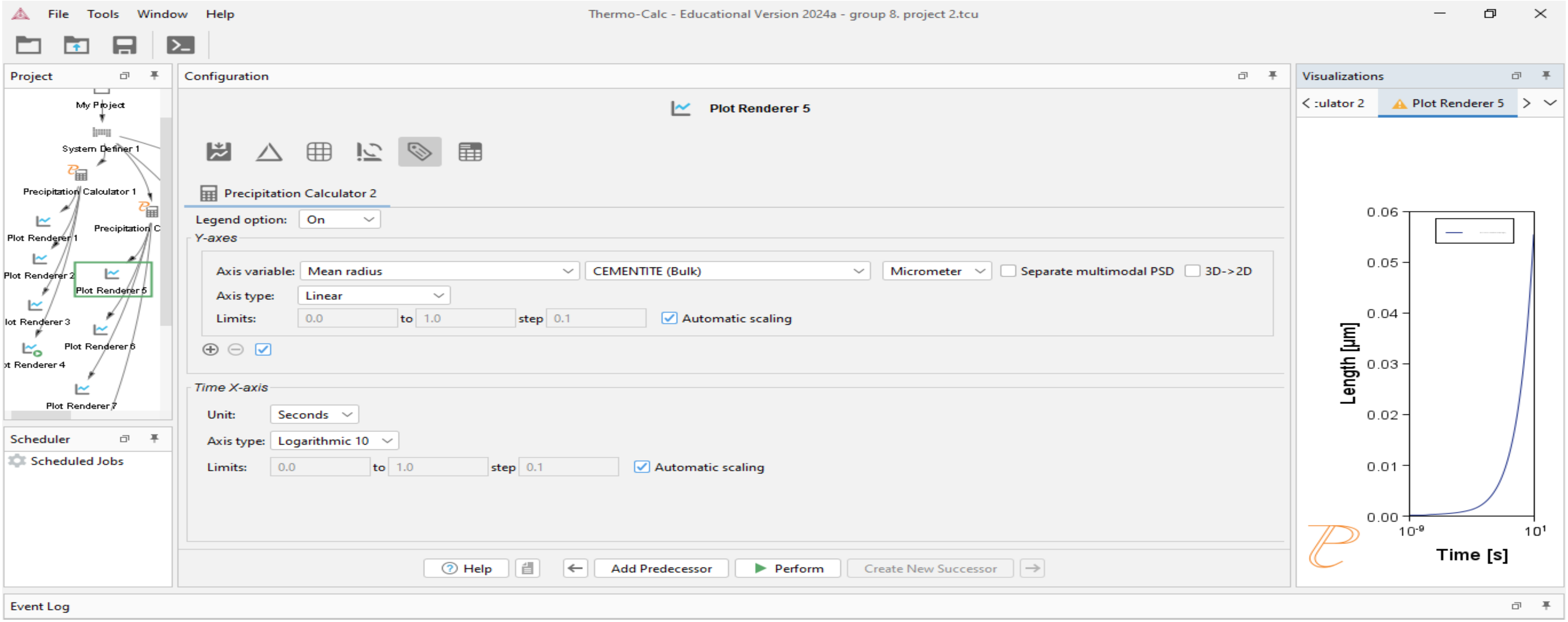


Figure 16: A schematic showing the legend option, with the X-axis representing time measured in seconds with a logarithm base 10 axis type and limits, and the Y-axis representing the mean radius of Cementite (Bulk) in micrometers with a linear axis type.

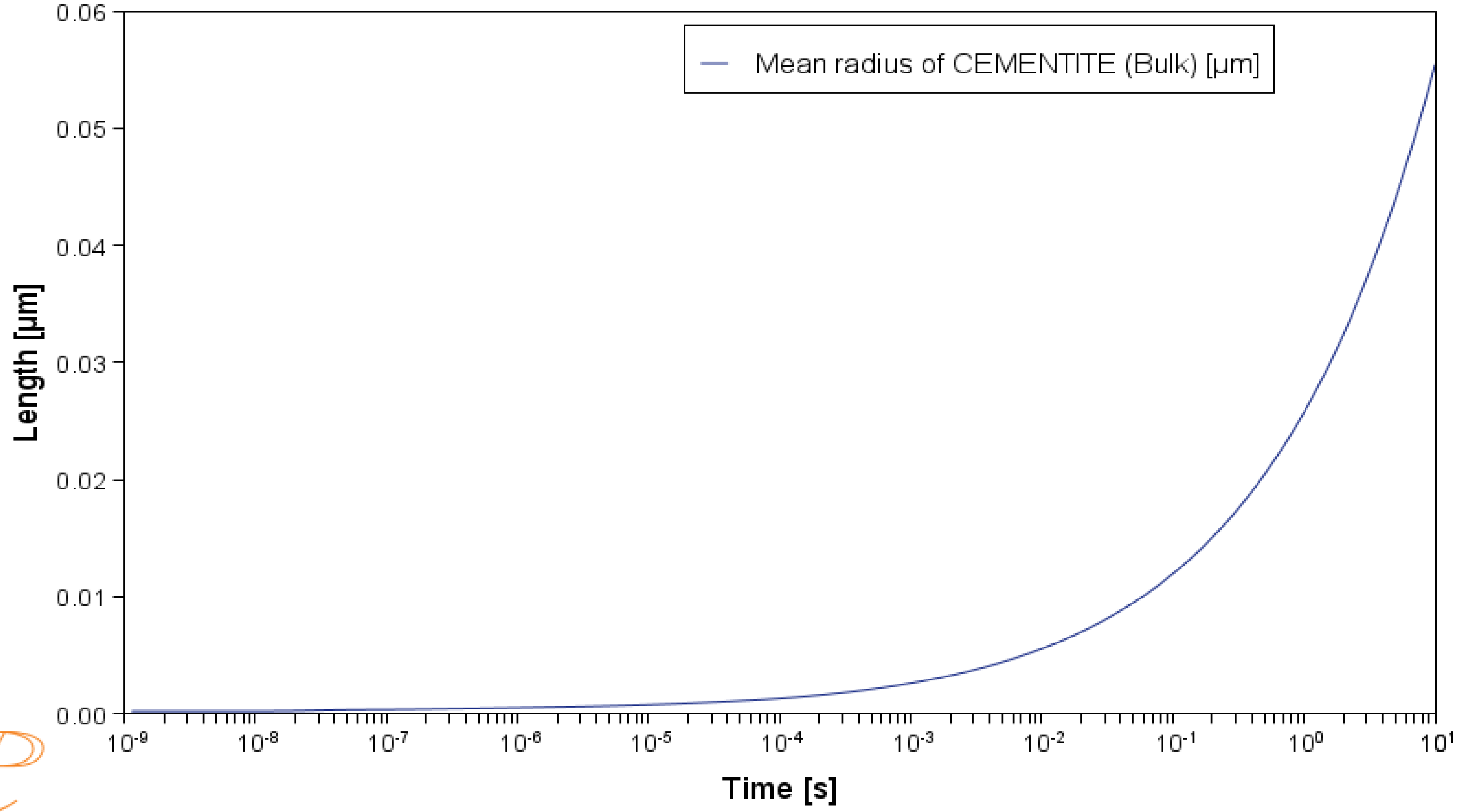


Figure 17. Mean radius of Cementite (Bulk) in the precipitate

The diagram shows the mean radius of cementite (Bulk) precipitates over time on a logarithmic scale. The x-axis represents time in seconds, ranging from 0.000000001 to 10 seconds, and the y-axis represents the radius in micrometers. Initially, the radius remains nearly constant, indicating minimal growth. As time progresses, particularly beyond 0.01 seconds, the radius starts increasing more rapidly, displaying an exponential growth pattern. This indicates that the precipitation process of cementite particles begins slowly but accelerates significantly as time passes, reflecting a transition from nucleation to a faster growth phase.

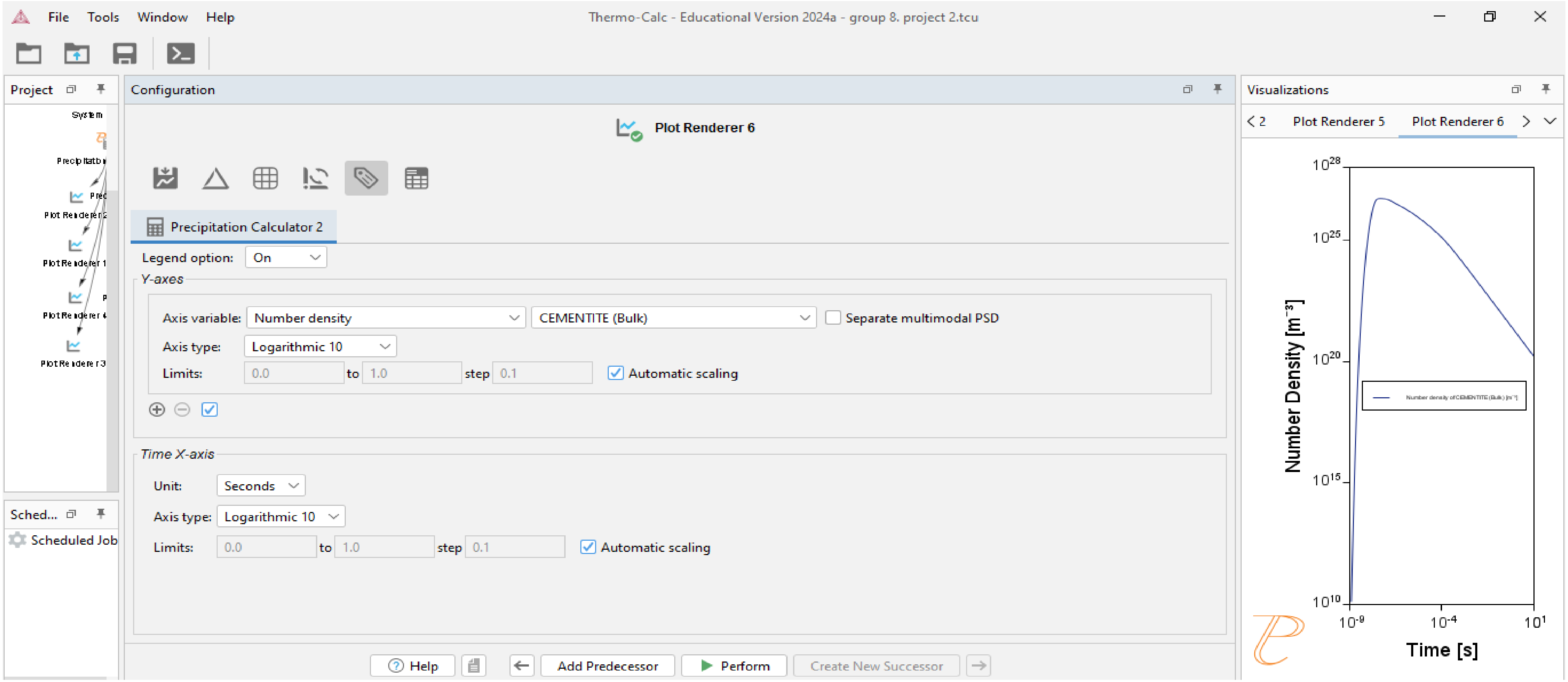


Figure 18: A schematic showing the legend option, with the X-axis representing time measured in seconds using a logarithmic base 10 scale, and the Y-axis representing the number density of cementite (bulk) using a logarithmic base 10 scale.

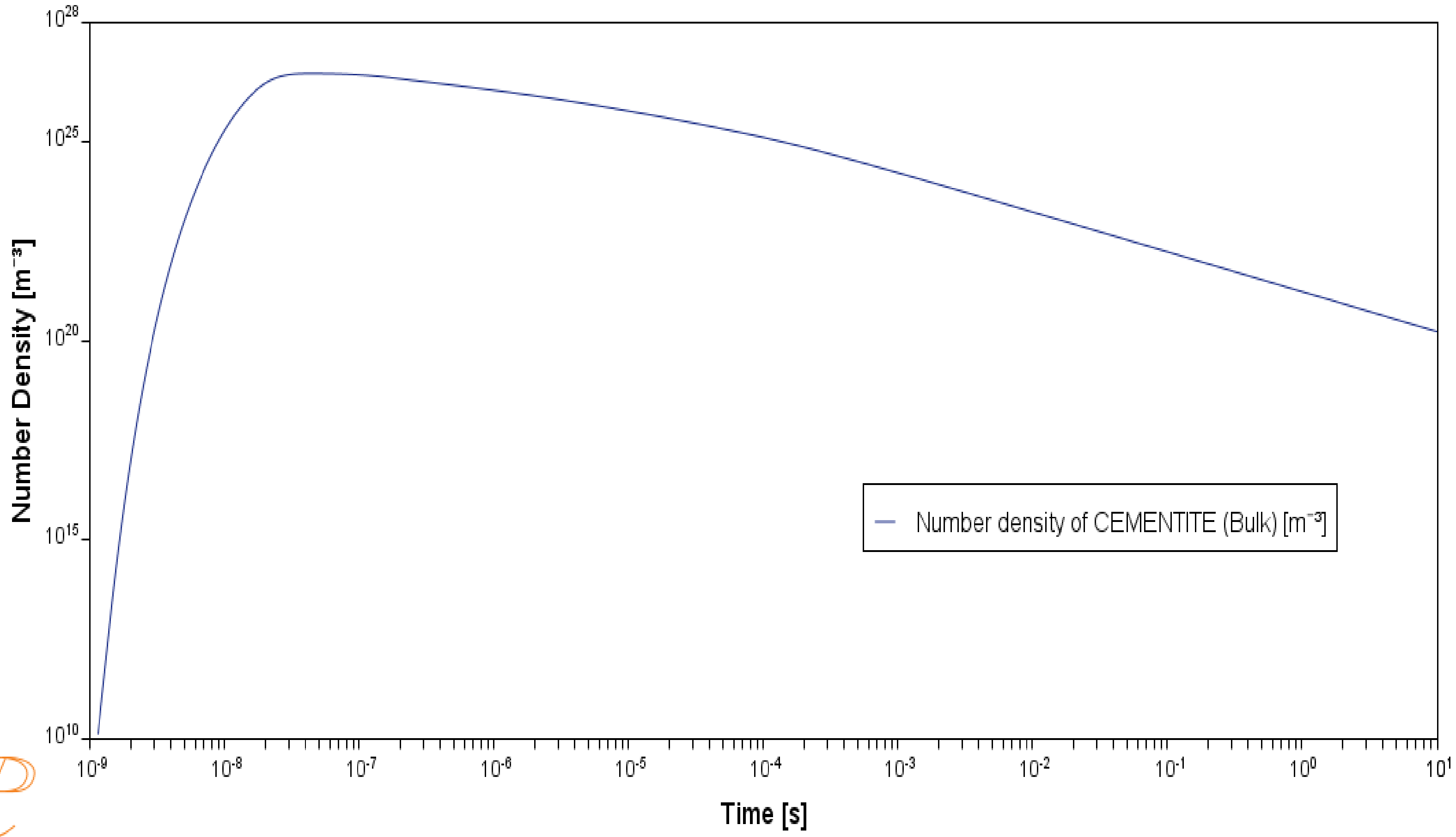


Figure 19. The number density of cementite as a function of time

The diagram shows the number density of cementite in bulk material as a function of time on a logarithmic scale. Initially, there is a rapid increase in number density, peaking around 0.0000001 seconds, indicating rapid nucleation and formation of cementite particles. Following the peak, the number density gradually declines, likely due to processes where larger particles grow at the expense of smaller ones, phase transformations, or dissolution, reducing the number of cementite particles over time. The graph illustrates the dynamic formation and stabilization behavior of cementite in the material.

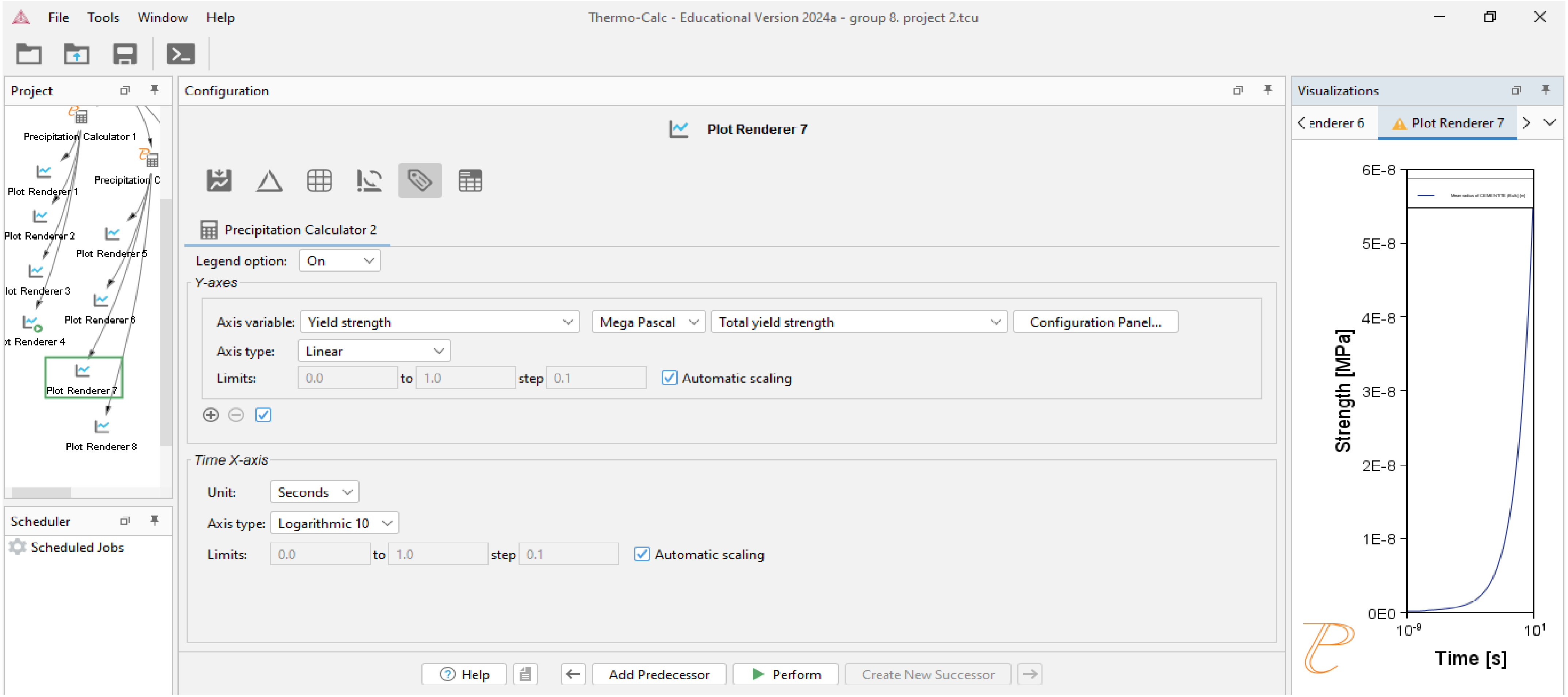


Figure 20: A schematic showing the legend option, with the X-axis representing time measured in seconds with a logarithm base 10 axis type and limits, and the Y-axis representing the yield strength of Cementite (Bulk) in megapascals with a linear axis type.

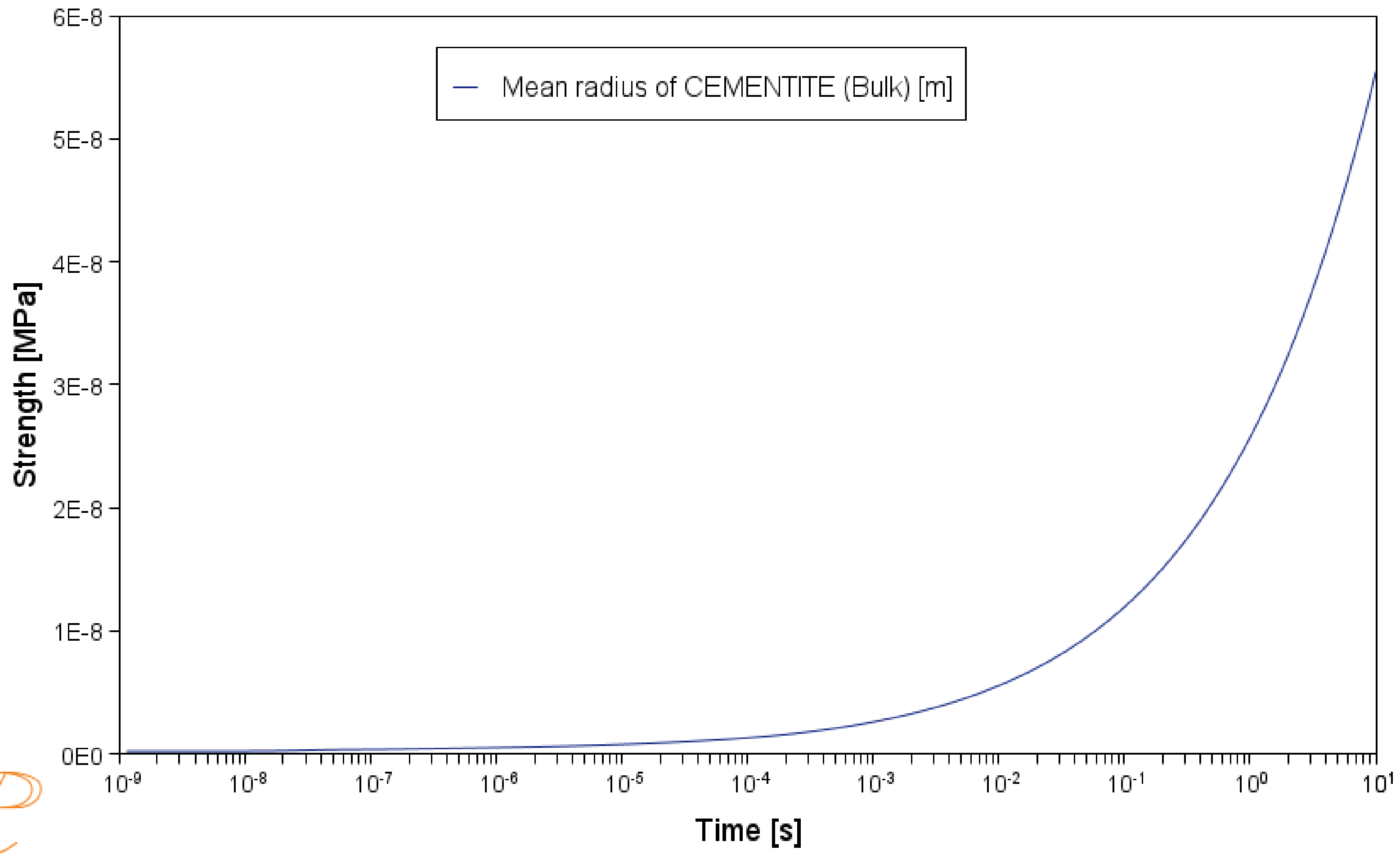


Figure 21. The trend of yield strength as a function of time.

The diagram illustrates the trend of yield strength as a function of time on a logarithmic scale. The x-axis represents time in seconds, ranging from 0.000000001 to 10 seconds, while the y-axis represents strength in megapascals (MPa). Initially, the yield strength remains very low and nearly constant, suggesting minimal changes in the material properties. As time progresses, particularly after 0.01 seconds, the yield strength begins to increase more rapidly, showing an exponential growth pattern. This trend indicates that the material's yield strength improves significantly over time, likely due to the ongoing precipitation and growth of cementite particles, which enhance the overall mechanical properties of the material

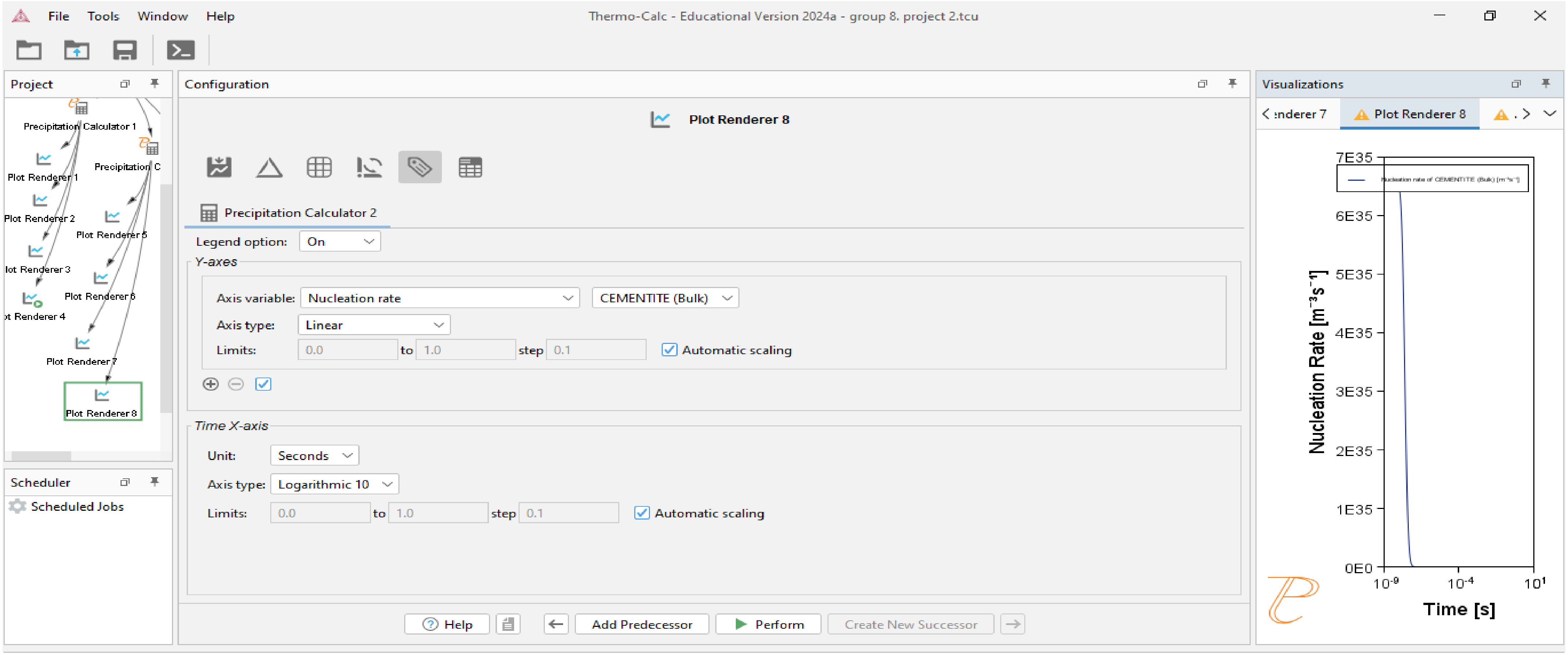


Figure 22: A schematic showing the legend option, with the X-axis representing time measured in seconds with a logarithm base 10 axis type and limits, and the Y-axis representing the nucleation rate of Cementite (Bulk) with a linear axis type.

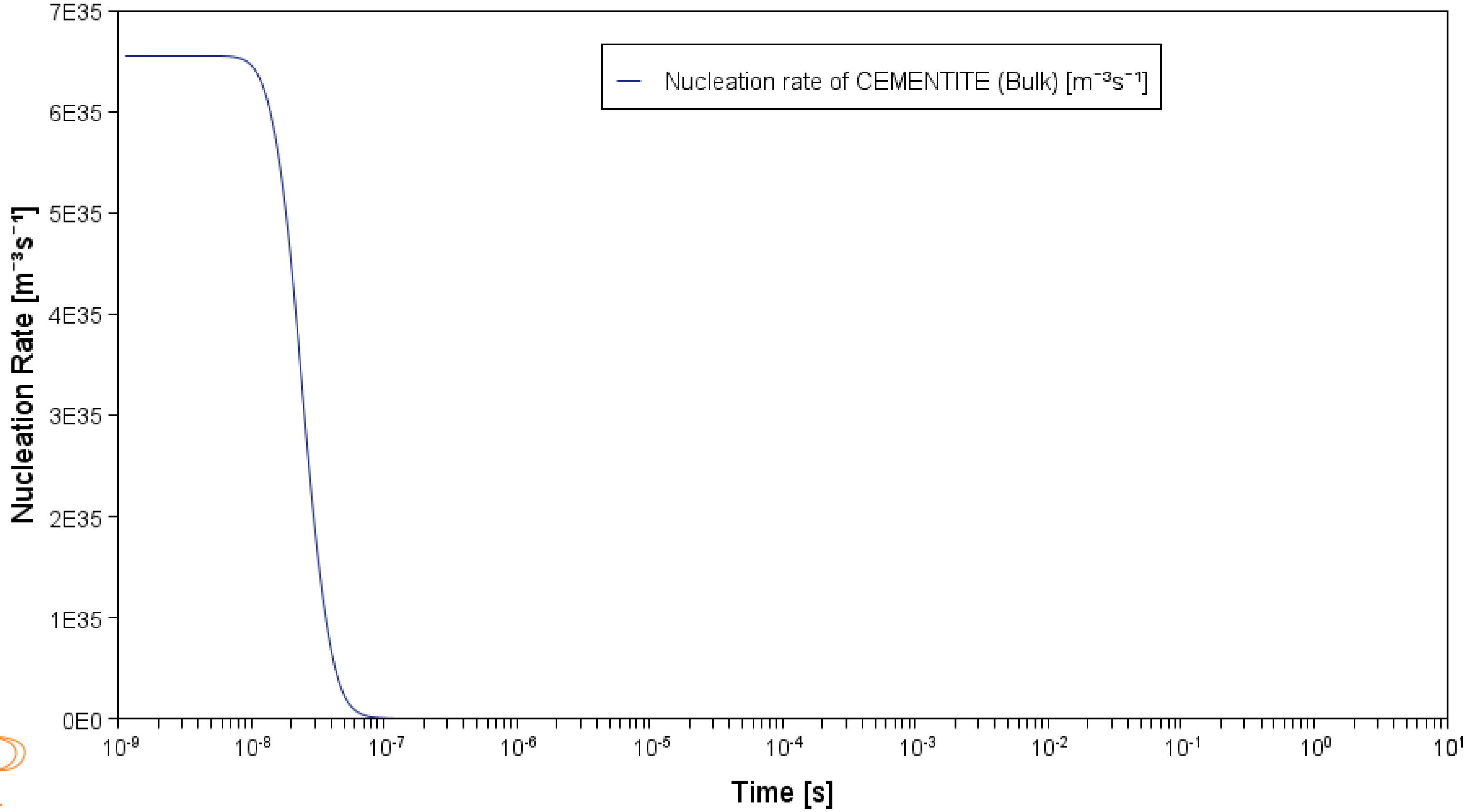


Figure 23. The Nucleation rate as a function of Time

The diagram illustrates the nucleation rate of cementite (Bulk) as a function of time on a logarithmic scale. Initially, the nucleation rate is extremely high, maintaining a value around 6.5E35 up to approximately 0.0000001 seconds. Beyond this point, the nucleation rate sharply declines and approaches zero around 0.0000001 seconds. This trend indicates an intense initial phase of nucleation where numerous new cementite particles form rapidly. Additionally, the nucleation rate drops off quickly, suggesting that nucleation events become rare as existing particles begin to grow.

COMMENT ON HOW ARE THE NUCLEATION RATE, THE AVERAGE PRECIPITATE SIZE, AND THE MECHANICAL PROPERTIES CORRELATED

In both cases, the nucleation rate, average precipitate size, and mechanical properties are interrelated through the dynamics of cementite precipitation and growth.

Nucleation Rate: At 300°C, the nucleation rate starts extremely high and drops sharply within microseconds, indicating rapid initial nucleation followed by a significant decrease as resources deplete or conditions become less favorable. At 600°C, a similar pattern is observed but at a higher nucleation rate. This rapid initial nucleation phase ends within nanoseconds, again showing a steep decline as nucleation resources are quickly exhausted.

Average Precipitate Size: At 300°C, the mean radius of cementite precipitates shows a slow initial increase, followed by a more rapid growth phase after 0.0001 seconds. This suggests a transition from nucleation-dominated to growth-dominated processes. At 600°C, the average precipitate size remains almost constant initially but then increases rapidly after 0.01 seconds. The higher temperature accelerates diffusion, leading to quicker and larger precipitate growth.

Mechanical Properties: The yield strength correlates with the growth of cementite particles. At 300°C, yield strength remains low initially but starts increasing more noticeably beyond 0.00001 seconds, as the precipitates grow and contribute to strengthening the material. At 600°C, the yield strength also stays low initially but begins to rise significantly after 0.01 seconds, corresponding to the faster growth of precipitates at higher temperatures.

Correlation: Higher nucleation rates at the onset lead to a rapid increase in the number of small precipitates. As these precipitates grow, their number density decreases due to coarsening, leading to an increase in the average precipitate size. The mechanical properties, particularly yield strength, are enhanced as precipitates grow. This is because larger and more numerous precipitates impede dislocation motion more effectively, thereby increasing the material's strength. The faster kinetics at 600°C result in quicker changes in both precipitate size and mechanical properties compared to 300°C, demonstrating the temperature-dependent nature of these processes.

COMMENT ON HOW DOES THE TEMPERATURE INFLUENCE THE PRECIPITATION PROCESS

Temperature influences the precipitation process by affecting nucleation rates, growth kinetics, and precipitate stability. At higher temperatures (600°C), atomic mobility and diffusion rates increase, leading to a rapid but short-lived nucleation phase followed by accelerated growth of larger precipitates, which enhances yield strength more quickly but can result in coarser precipitates. At lower temperatures (300°C), nucleation occurs more slowly, and growth kinetics are reduced, resulting in smaller, more numerous precipitates that grow gradually. This slower process leads to a steadier increase in yield strength due to a finer precipitate distribution that effectively impedes dislocation motion over a longer period.

END

Politecnico di Torino

1859