

Alloy design toolkit documentation

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Alloy design toolkit is a GUI-driven environment that integrates thermodynamic/kinetic calculations with exploratory search to support alloy design in Fe-based alloys. It exposes six individual models—phase fractions & compositions, martensite/retained-austenite (Ms, Fm, RA), stacking fault energy (SFE), multi-objective optimization (NSGA-II-style), PRISMA-based precipitation kinetics, and geometric-mean (GM) ranking for optimal annealing time—each runnable standalone or sequenced end-to-end via an automated workflow. The workflow reads composition grids, evaluates phase stability and SFE, filters options under user constraints, simulates precipitation, and ranks time–temperature choices; results are exported to a multi-sheet Excel file that summarizes the overall process and highlights the top candidate alloys.

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1. Standalone scripts (individual models)

This section (shown in Figure 1) of the toolkit allows users to run individual computational models independently of the full automated workflow. Each button corresponds to a specific calculation script located in the “standalone scripts” directory.

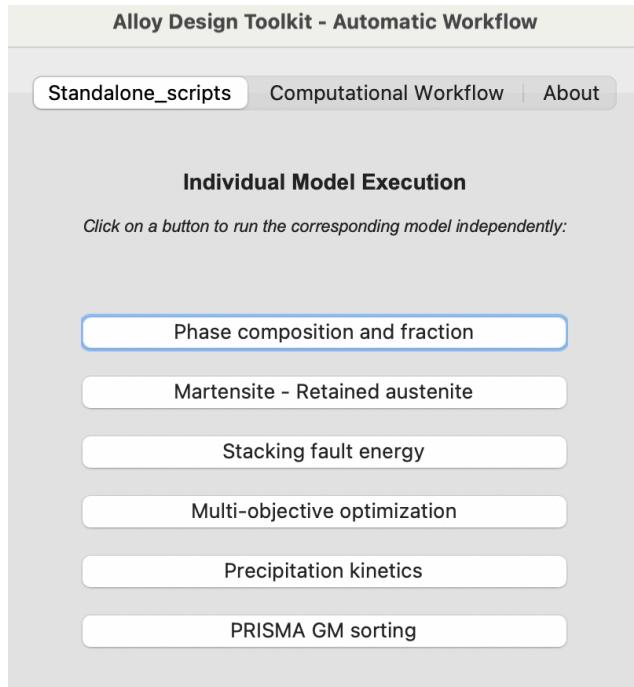


Figure 1 Standalone scripts (individual models) tab

- **Phase composition and fraction:** Runs the script “1 phase fraction and composition.py” to perform thermodynamic calculations for phase fractions and compositions across a range of temperatures and compositions.
- **Martensite - Retained austenite:** Runs the script “2 retained austenite model.py” to calculate the Martensite Start (Ms) temperature, martensite fraction (Fm), and retained austenite (RA) fraction based on austenite composition and quenching temperature.
- **Stacking fault energy:** Runs the script “3 SFE model.py” to calculate the Stacking Fault Energy (SFE) of austenite based on chemical composition, temperature, and other physical parameters.
- **Multi-objective optimization:** Runs the script “4 MOO algorithm.py” to perform multi-objective optimization (using NSGA-II principles) on previously calculated data (phase fractions, RA, SFE) to find optimal alloy compositions and processing temperatures based on defined objectives and constraints.
- **Precipitation kinetics:** Runs the script “5 Precipitation kinetics.py” to simulate precipitation kinetics using the TC-PRISMA module for given alloy compositions and annealing conditions.
- **PRISMA GM sorting:** Runs the script “6 PRISMA GM sorting.py” to process time-series precipitation data (from PRISMA), normalize selected objectives, calculate an overall score using the geometric mean (GM), and rank the time steps for each alloy to determine the optimal annealing time.

1.1. Phase fraction and composition calculation model

This script performs thermodynamic calculations using TC-Python to determine phase fractions and compositions as a function of temperature for various alloy compositions. It uses parallel processing to speed up calculations across different compositions and resamples the results onto a user-defined temperature grid.

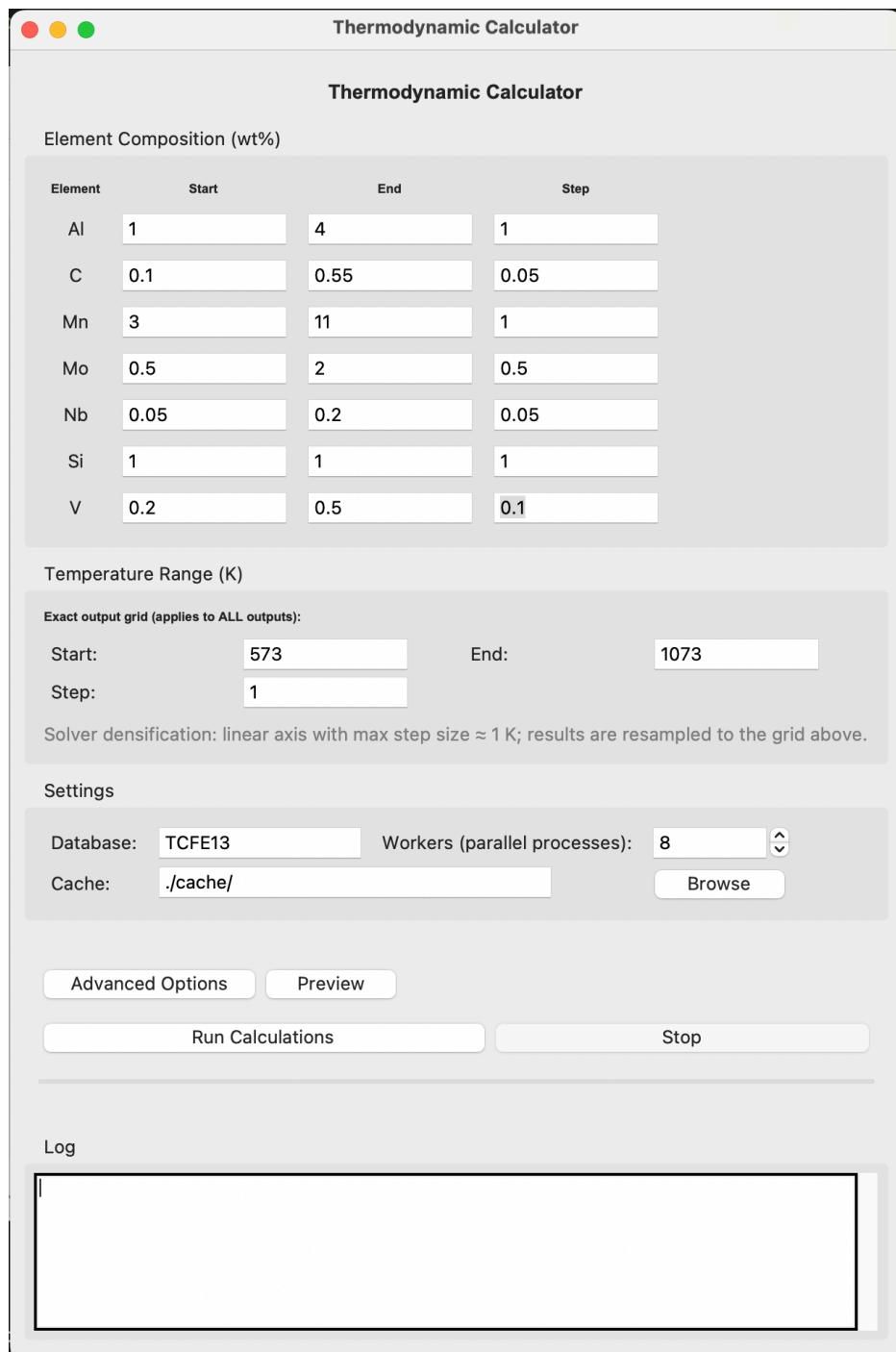


Figure 2 Phase fraction and composition calculator GUI

1.1.1. Element composition

Define the composition space by specifying the Start, End, and Step values (in wt.%) for each alloying element. Fe is automatically calculated as the balance.

1.1.2. Temperature range

Set the Start, End, and Step temperature (in Kelvin) for the calculations. The results are resampled to this exact grid. The solver densifies the calculation steps internally to ensure accuracy.

1.1.3. Settings

Configure the thermodynamic Database (e.g., TCFE13), the number of parallel Workers (processes), and the location of the Cache folder for storing intermediate calculation results.

1.1.4. Advanced options

This section allows for more detailed configuration through three tabs:

- Alloying elements: Select the specific elements (besides Fe) to be included in the thermodynamic system using a periodic table interface as shown in Figure 3.
- Phases: Choose the phases (e.g., FCC_A1, BCC_A2, CEMENTITE) for which fractions and compositions should be calculated and exported as shown in Figure 4.
- Results: Select whether to export Phase Fraction (volume fraction) and/or Phase Composition (mass fraction of elements within each phase) as shown in Figure 5.



Figure 3 Advanced options - alloying elements tab



Figure 4 Advanced options – phases selection tab

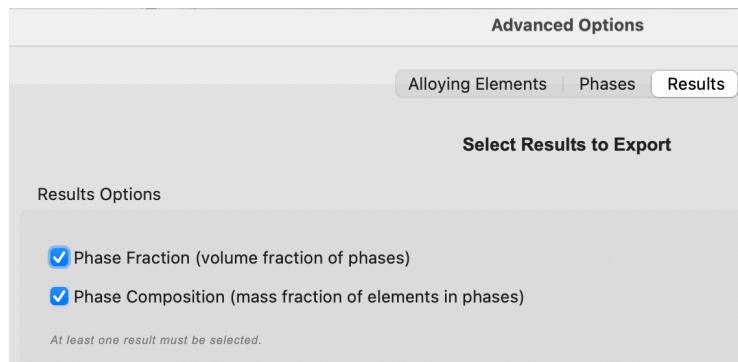


Figure 5 Advanced options – required results tab

1.2. Retained austenite – martensite fraction prediction model

The tool calculates the Ms temperature, Fm, and RA fraction. It reads phase calculation results from an Excel file, applies empirical formulas, and appends the results (Ms, Fm, RA) back to the same file.

- File Selection: Select the Excel file containing the phase calculation results. The file must include specific columns like "Mass_fraction_C_in_FCC_A1, FCC_A1_Fraction" etc., as listed in the "Information" tab.
- Calculation Parameters: Enter the Quenching Temperature (°C), typically room temperature (e.g., 25°C), used in the Fm calculation.
- Run Calculation: Click "Calculate and Save Results" to perform the calculations for all rows in the selected Excel sheet and save the output back to the file.

1.3. Stacking fault energy model

This application calculates the Stacking Fault Energy (SFE) for austenitic steels based on their chemical composition (in wt%) and other parameters. It supports single calculations, batch processing via Excel import, and parametric studies over composition ranges.

Composition Inputs: Enter the weight percentages for C, Mn, Si, Al, Mo, N, Cr, Ni, and Cu.

Calculate SFE: Computes the SFE for the entered composition using the current advanced parameters. The result is displayed at the bottom as shown in Figure 6.

Advanced Options: Opens a dialog to adjust parameters like Interfacial Energy (σ), Grain Size, Lattice Parameter (a), and Temperature (K) used in the SFE calculation.

Chemical Composition Range: Opens a dialog for performing parametric studies. Users can define Start, End, and Step values for each element as shown in figure Figure 8. The tool calculates SFE for all combinations and saves the results to a new Excel file.

Import from Excel: Allows batch processing by reading compositions from an Excel file. The file needs specific columns (e.g., Mass_fraction_C_in_FCC_A1 or simple element symbols like C). SFE is calculated for each row, and the results are saved to a new Excel file.

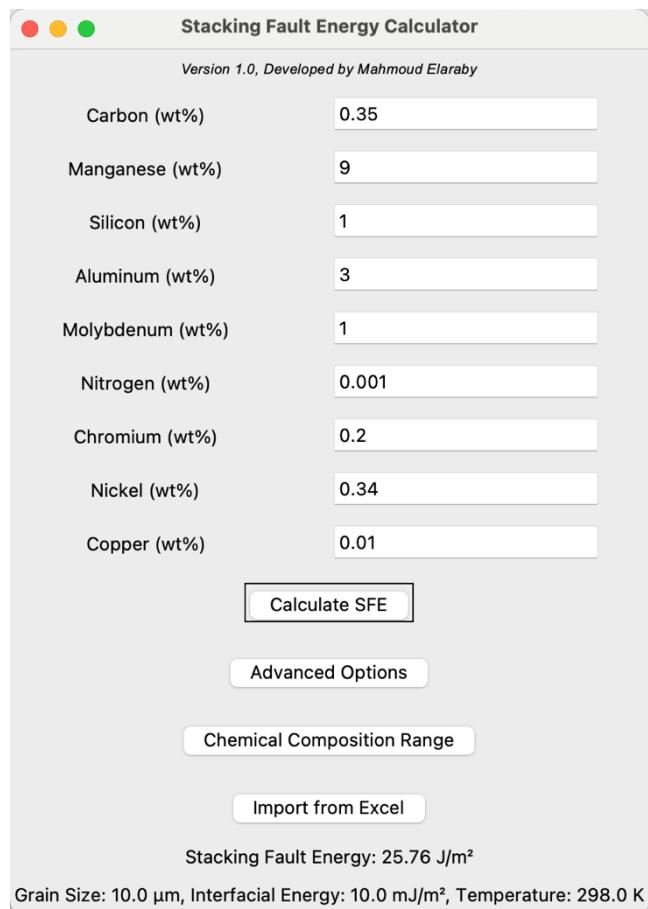


Figure 6 Stacking fault energy calculation model GUI

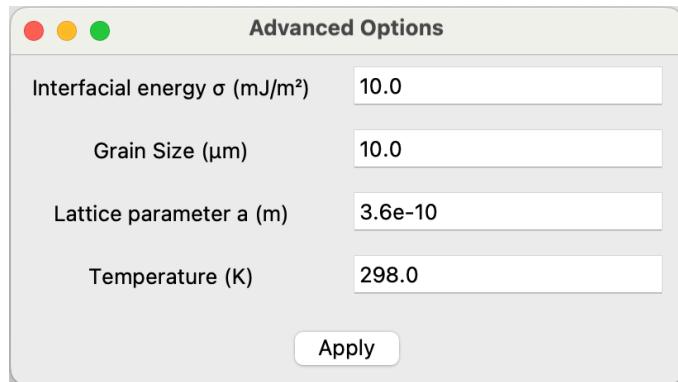


Figure 7 Advanced options of the SFE model

Chemical Composition Range			
C Start:	0.0	C End:	0.0
Mn Start:	0.0	Mn End:	0.0
Si Start:	0.0	Si End:	0.0
Al Start:	0.0	Al End:	0.0
Mo Start:	0.0	Mo End:	0.0
N Start:	0.0	N End:	0.0
Cr Start:	0.0	Cr End:	0.0
Ni Start:	0.0	Ni End:	0.0
Cu Start:	0.0	Cu End:	0.0
Current Advanced Parameters:			
Grain Size: 10.0 µm, Interfacial Energy: 10.0 mJ/m ² , Temperature: 298.0 K			
<input type="button" value="Calculate"/>			

Figure 8 Calculation of SFE for a chemical composition range

1.4. Multi-objective optimization algorithm

This tool applies multi-objective optimization techniques, inspired by NSGA-II, to discrete data points generated from previous calculation steps (Ms, RA, SFE, and ΔT) as shown in Figure 9. It aims to find optimal alloy compositions and intercritical annealing temperatures that balance multiple objectives (e.g., maximizing RA, SFE, ΔT while minimizing Ms) subject to user-defined constraints.

- **Data loading:** Load the input data from an Excel file containing results from prior steps (Phase Calc, RA Calc, SFE Calc). The required columns include element compositions, Temperature, Ms, Ra, SFE, Fm, and Cementite fraction.
- **Alloy design constraints:** Set the acceptable ranges and limits for key properties: Ms min/max ($^{\circ}\text{C}$), RA min/max, SFE min/max (mJ/m^2), Min ΔT ($^{\circ}\text{C}$) (minimum required processing window width), and Cementite limit (maximum allowed fraction).
- **Process MOO (auto GM ranking):** Executes the optimization process:

- 1) Filters the input data based on the defined constraints.
- 2) Calculates the processing window (ΔT) for each valid composition.
- 3) Selects an optimal temperature (T_{opt}) within the valid window.
- 4) Performs non-dominated sorting to assign ranks (Pareto fronts).
- 5) Calculates the crowding distance to differentiate solutions within the same rank.
- 6) Sorts solutions by rank (ascending) and crowding distance (descending).
- 7) Applies GM ranking to the top 20 solutions based on normalized objective values to provide an additional single-score ranking.

- **Plot Pareto Front:** Visualizes the trade-offs between different pairs of objectives for the top-ranked solutions (typically rank 1, 2, 3).
- **Export Results:** Saves the ranked optimization results, including composition, T_{opt} , objectives, Rank, Crowding distance, and GM scores/ranks, to an Excel file. Multiple sheets might be created (e.g., All Results, Pareto Front, GM Ranked).

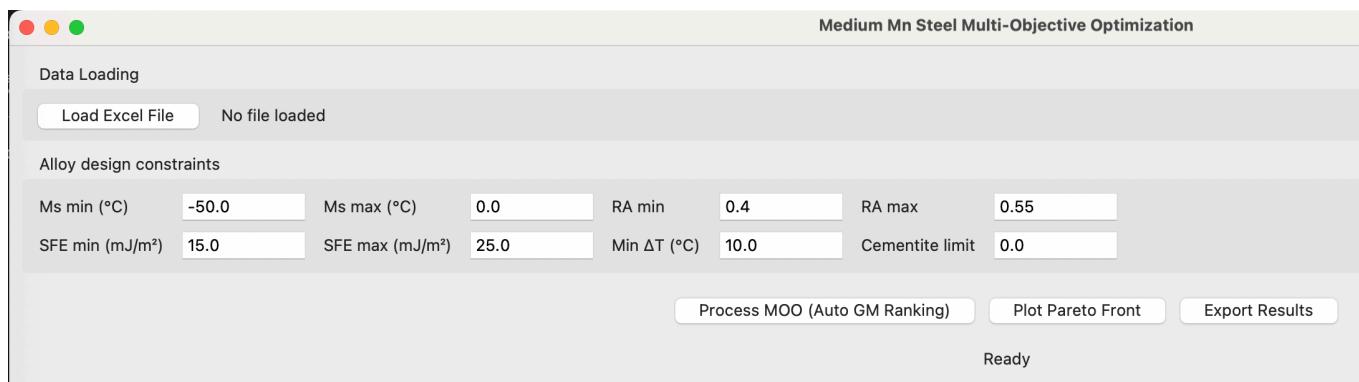


Figure 9 Multi-Objective Optimization model GUI

1.5. Precipitation kinetics (PRISMA)

This application provides a graphical interface for running isothermal precipitation simulations using the TC-Python PRISMA module as shown in Figure 10, primarily for Fe-based alloys. It allows users to load alloy compositions from an Excel file, configure simulation parameters, and export detailed time-series results.

1.5.1. Input and output files

Specify the Input Excel file containing alloy compositions (one per row, including a 'Temperature' column in °C) and the desired Output Excel file name for saving simulation results.

1.5.2. Precipitation parameters

Define the Simulation Time (seconds), the name of the matrix phase (e.g., FCC_A1), and the name of the precipitate phase (e.g., FCC_A1#2 or CEMENTITE). The temperature is read from the input Excel file for each composition.

1.5.3. Database settings

Specify the Thermodynamic DB (e.g., TCFE13), the Kinetic DB (e.g., MOBFE8), and the Cache Folder location.

1.5.4. Advanced options

Access additional settings as shown in Figure 11:

- **Alloying elements:** Select the elements to include in the calculation system.
- **Nucleation sites:** Choose the primary site for precipitate nucleation (e.g., Bulk, Grain boundaries, Dislocations).
- **Growth rate model:** Select the model governing precipitate growth (e.g., Simplified, General, PE_AUTOMATIC).
- **Results to calculate:** Choose which time-dependent results to compute and export (e.g., Volume fraction, Mean radius, Number density, Nucleation rate, Matrix composition, Precipitate composition).

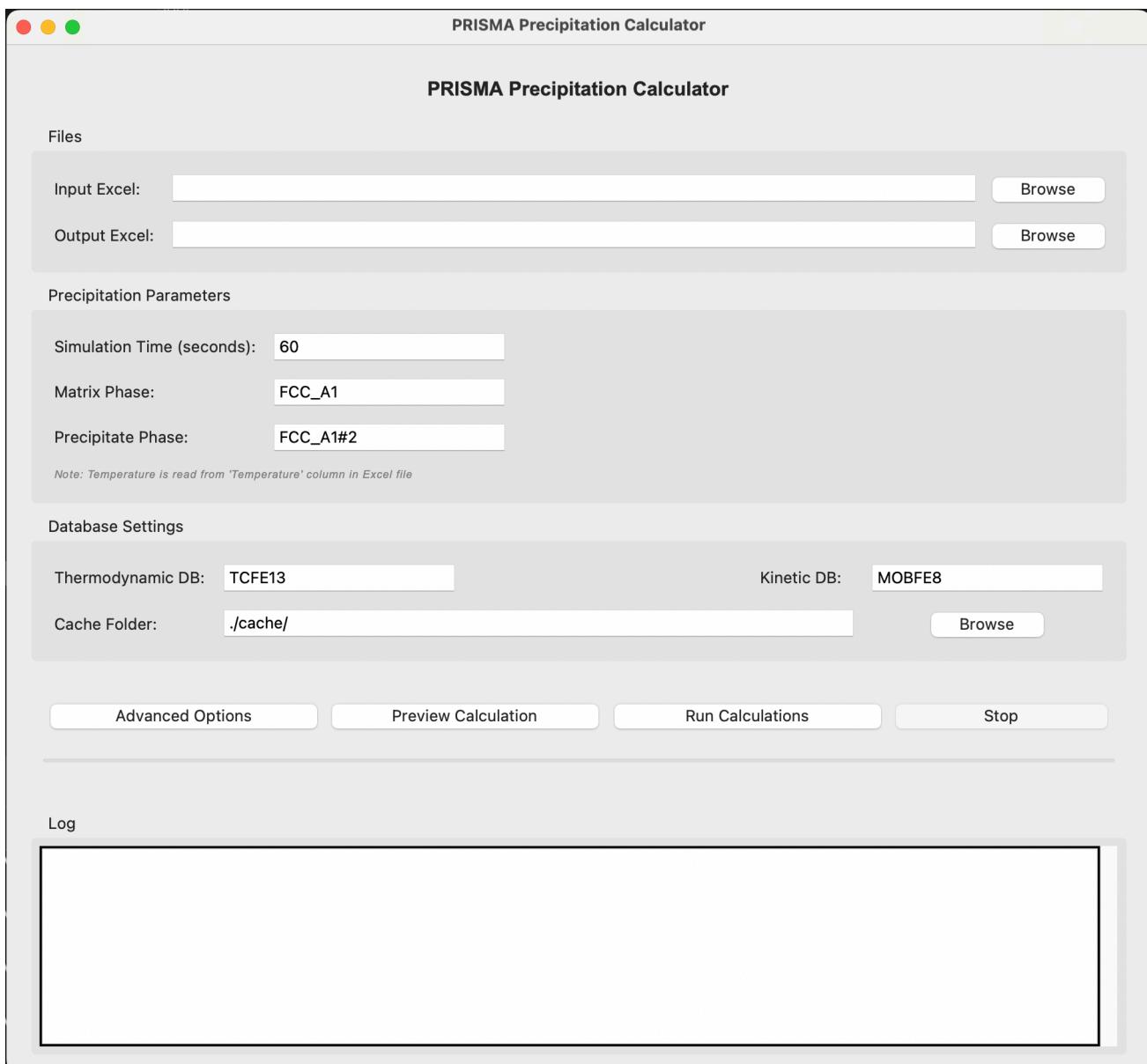


Figure 10 Precipitation (PRISMA) kinetics model GUI

1.6. Optimal annealing time (GM sorting)

This tool processes precipitation data (generated by the precipitation script) for individual alloy compositions. It normalizes user-selected objectives (e.g., time, mean radius, number density, volume

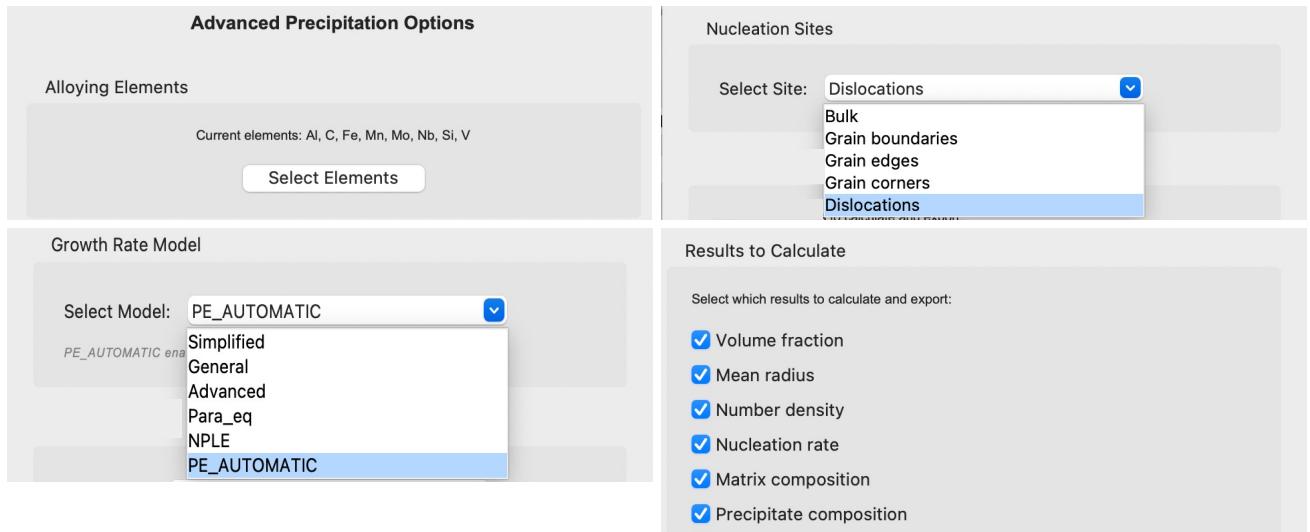


Figure 11 Advanced options of the precipitation module

fraction, matrix composition) and calculates an overall score using the GM for each time step, as shown in Figure 12. Ranking these scores identifies the optimal annealing time (corresponding to the highest score) for each distinct alloy composition present in the input file.

Input File: Load an Excel file containing the time-series precipitation data. It must include an identifier column (like 'Composition' or 'GM_Rank') and columns for the objectives to be evaluated.

Select objectives for ranking : Checkboxes allow the user to select which calculated objectives should contribute to the Overall Score calculation. The goal (minimize or maximize) for each objective is displayed.

Process data: Triggers the normalization, Geometric Mean calculation, and ranking process for each unique alloy composition found in the loaded data.

Export to Excel: Saves the processed data, including normalized columns, Overall Score, and Rank_within_Alloy, to a new Excel file.

Results display: A table shows the processed data, sortable by clicking column headers. It includes the original data, normalized objective values (0-1), the calculated Overall Score, and the rank of each time step within its specific alloy group.

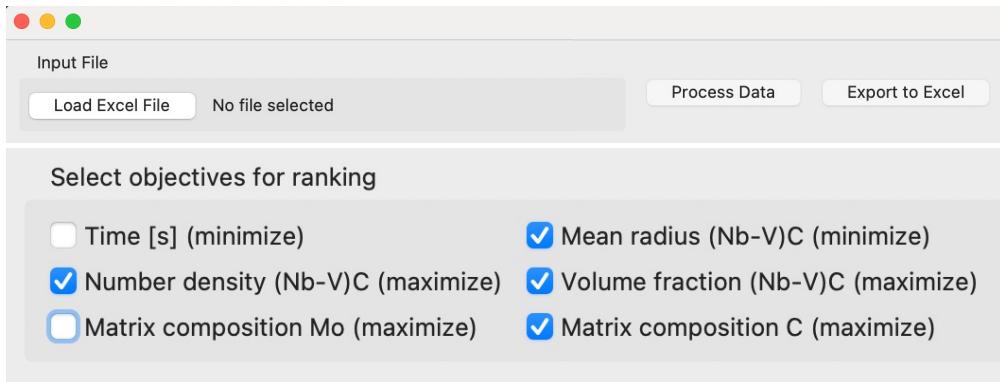


Figure 12 Optimal annealing time prediction (ranking precipitation data via GM)

2. Computational workflow (automated calculations)

This tab arranges the sequential execution of the entire alloy design workflow, running the core calculation modules one after another.

Workflow steps: Displays the main steps involved in the automated workflow. Clicking the button next to each step opens its specific configuration dialog:

- 1) **Phase calculations:** Configure composition ranges, temperature, phases, database, and parallel workers.
- 2) **Stacking fault energy:** Configure SFE calculation parameters like interfacial energy, grain size, and temperature.
- 3) **Multi-objective optimization:** Set design constraints (Ms, RA, SFE ranges, ΔT , Cementite limit) and quenching temperature.
- 4) **Precipitation kinetics:** Configure PRISMA simulation time, phases, databases, growth model, and nucleation site.
- 5) **Optimal annealing time:** Configure the objectives used for Geometric Mean sorting of precipitation results.

Run workflow: Starts the execution of the entire workflow sequence. A separate thread is used for the calculations to keep the GUI responsive.

Stop: Requests the workflow to stop after completing the current step.

Progress bar: Shows the overall progress of the workflow.

Workflow log: Displays status messages, progress updates, warnings, and errors generated during the workflow execution.

After the workflow completes successfully, the computational data is exported to an Excel file "Alloy_design_result.xlsx", which is composed of five sheets having the results of the previous five steps, finally recommending the top 20 alloys among all the investigated alloys.

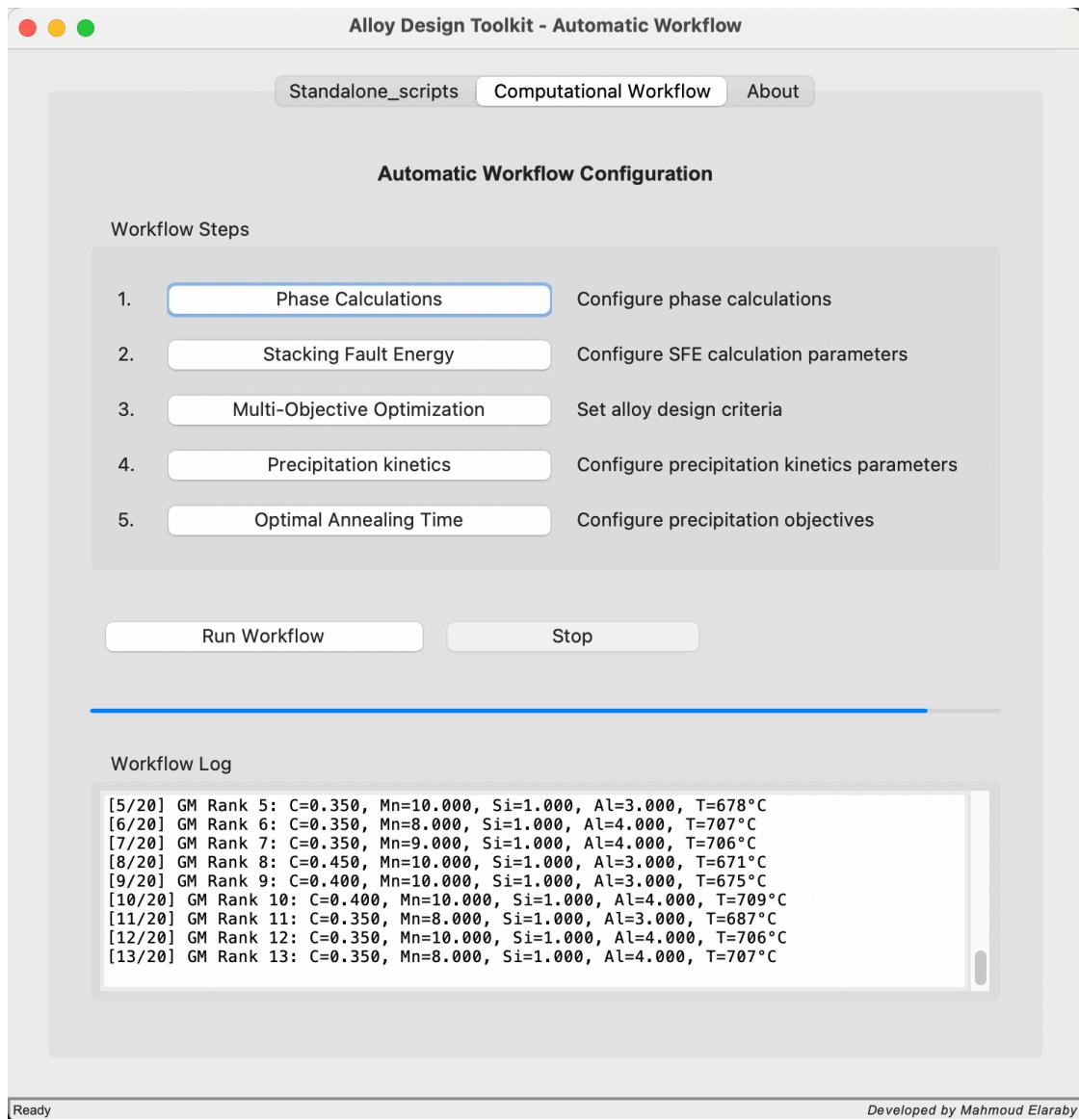


Figure 13 Computational workflow (automatic process) tab