The Alloy Optimization Software (TAOS)

User Manual

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Contents

1. Description

The Alloy Optimization Software (TAOS) has been developed at LLNL to be a powerful, user-friendly tool that allows for computational design of optimal alloys on commodity stand-alone computer hardware. It does not require users to have domain expertise in computational materials science.

TAOS allows users to design new materials with a targeted property (e.g., melting temperature, freezing range, phases formed) under applied constraints (e.g., phases to avoid, minimum melting temperature) in minutes to hours (depending on the constraint optimization criteria). Its intuitive graphical user interface (GUI) permits rapid screening of desired alloy compositions from a large multidimensional composition space down to a manageable number of experimental targets.

TAOS is based on the use of CALPHAD (CALculation of PHAse Diagrams) thermodynamic databases, integrates the PyCalphad thermodynamic engine to work as a self-consistent software with unencrypted databases, and automatically interacts with the Thermo-Calc software and commercial databases through TC-Python (being provided by www.thermocalc.com). Note that Thermo-Calc products are not included in TAOS.

2. System Requirements

Windows: Windows 10 (64-bit) or above

Mac: Mac OS X 11.7 (Big Sur) and above

3. Thermodynamic Software Compatibilities

TAOS is compatible with PyCalphad (included in the TAOS distribution) and TC-Python. Coupling TC-Python to TAOS can be done in the Preferences menu:

1. Switch Thermodynamic Software to TC-Python and click "Configure software…"
2. TAOS will attempt to find the Thermo-Calc SDK folder based off default installation paths. If it cannot find the SDK folder, the folder can be set with the Browse button.
    a. Windows: C:\Users\<Username>\Documents\Thermo-Calc\202xx
    b. MacOS: /Users/Shared/Thermo-Calc/202xx
    c. Note: On MacOS, the following environment variables need to be defined:
        i. TC2xx_HOME=/Applications/Thermo-Calc-202xx.app/Contents/Resources
        ii. If using a license server: LSHOST=<name of license server>
        iii. If using a node-locked license:
            1. LSHOST=NO-NET
            2. LSERVRC=/Users/Shared/Thermo-Calc/lservrc
        iv. More information can be found in the TC-Python documentation.
3. Click "Ok" on the Configure Software window and "Ok" on the Preferences window. This will couple the TC-Python module to TAOS.

4. Full Version Features

The full version includes compatibility with any PyCalphad and Thermo-Calc databases and access to the following properties:

- Composition
- Melting temperatures (*liquidus, solidus*)
- Solidification range (*equilibrium or Scheil*)
- Phase fractions at solidification (*equilibrium or Scheil*)
- Phase summation at solidification (*equilibrium or Scheil*)
- Phase fractions (*at absolute temperature or fraction of equilibrium solidus*)
- Phase summation (*at absolute temperature or fraction of equilibrium solidus*)
- Number of Elements
- Composition Summation
- Growth Restriction Factor
- Partition Coefficient
- Cracking Index

5. Demo Version Features

The demo version includes the same features as the full version with the following exceptions:

- The composition summation property, growth restriction factor, partition coefficient and cracking index properties are disabled.
- Database and project loading is limited to the following databases (these are included in the TAOS distribution in the "demos" folder):
    - AlCuSi_Hal2015.tdb
        - From: B. Hallstedt, J. Grobner, M. Hampl and R. Schmid-Fetzer, "Calorimetric measurements and assessment of the binary Cu-Si and ternary Al-Cu-Si phase diagrams" *Calphad* 53 (2016) p. 25-38. https://doi.org/10.1016/j.calphad.2016.03.002
    - FeCrC_Khvan2013.tdb
        - From: A. Khvan, B. Hallstedt and C. Broeckmann, "A thermodynamic evaluation of the Fe-Cr-C system" *Calphad* 46 (2014) p. 24-33. https://doi.org/10.1016/j.calphad.2014.01.002
    - AlCrNi_Dupin2001.tdb
        - From: N. Dupin, I. Ansara and B. Sundman, "Thermodynamic re-assessment of the ternary system Al-Cr-Ni" *Calphad* 25 (2001) p. 279-298. https://doi.org/10.1016/S0364-5916(01)00049-9

6. Input/Output

Project files (.taos)

- An optimization problem definition can be saved and loaded for later running or modifying the problem.
- The project file will save the following information:
    - Database
    - List of active elements
    - List of suspended phases
    - Units
    - Objective
    - Constraints
    - Optimizer Options
- Note: the project file is agnostic to the thermodynamic software and can be loaded regardless of the current active software given that the database is compatible.
- Note: If the database cannot be loaded (either the file path is wrong or the database is not compatible with the thermodynamic software), then the user will be prompted to load a replacement database to either correct the file path or use a compatible database for the current active software. If the replacement database is found to not be compatible with the rest of the project, then loading will be cancelled.
- Note: If for any reason, any of the units, objectives, constraints or optimizer options cannot be loaded, the user will be notified of what was not loaded in the output window.

Optimization output (.txt)

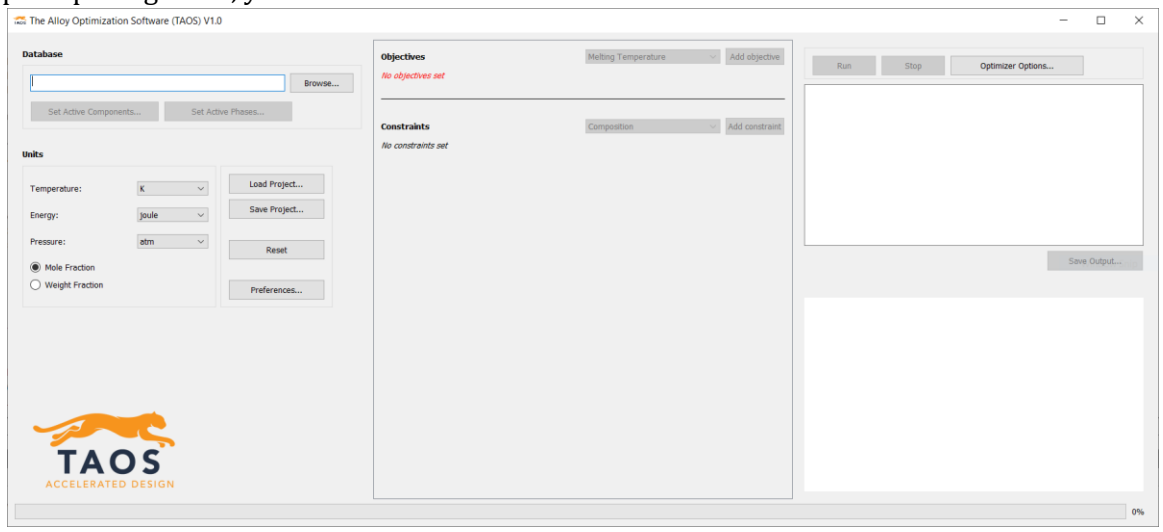
- Results of the optimization can be saved using the "Save Output" button.
- The following information will be saved:
    - Database
    - Active Elements
    - Suspended Phases
    - Problem Definition
        - Objective
        - Composition limits
        - Constraints (all constraints as read by the optimizer will be shown)
    - Optimization Results
        - Final composition
        - Objective value
        - Constraint values
    - Optimization History
        - This will list all black box evaluations which will include the composition, objective, and all constraints. Note: Sum1 and Sum2 columns are here by default to constrain the overall alloy composition to be equal to unity. The other constraint label will correspond to the label in the Problem Definition section.

7. Examples

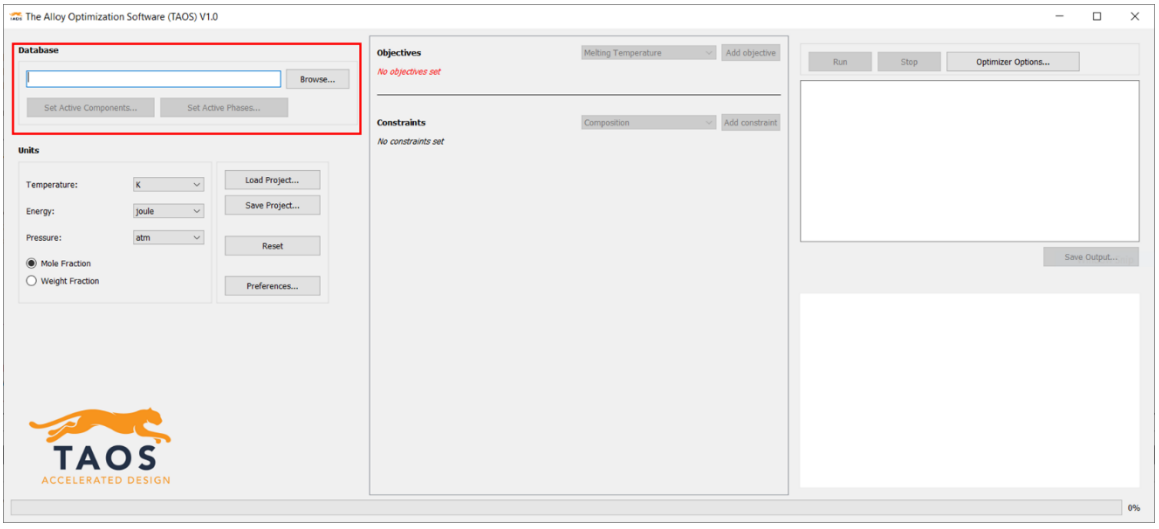
7.1. Example – Unconstrained Optimization (Al-Cu-Si)

Problem: *minimize* *Liquidus*

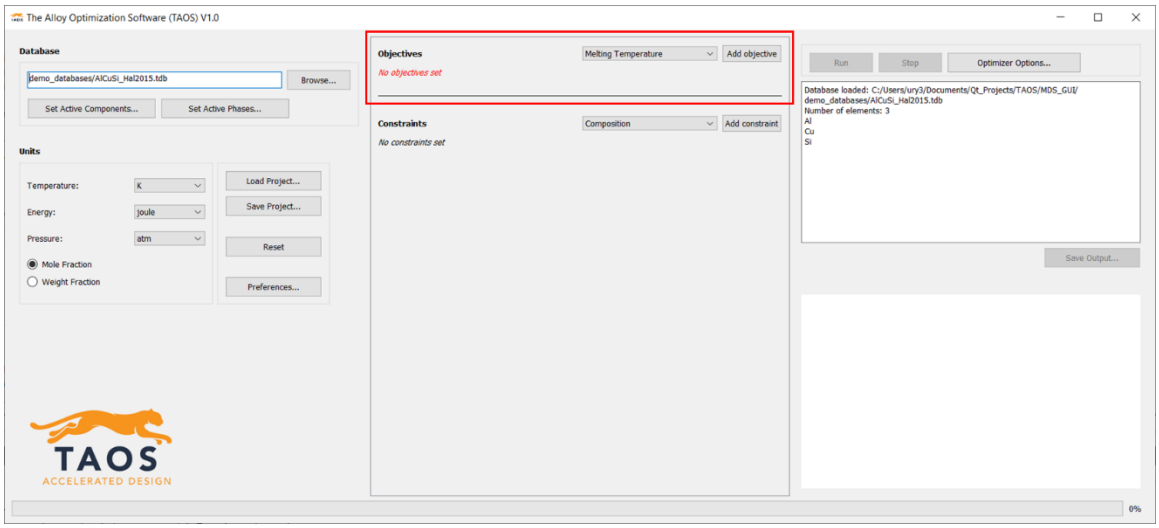
1. Upon opening TAOS, you should see this screen.

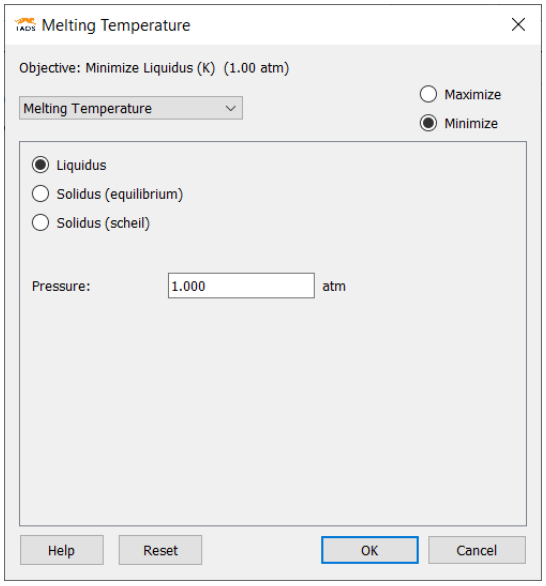


2. Load the database AlCuSi_Hal2015.tdb from the demos folder.

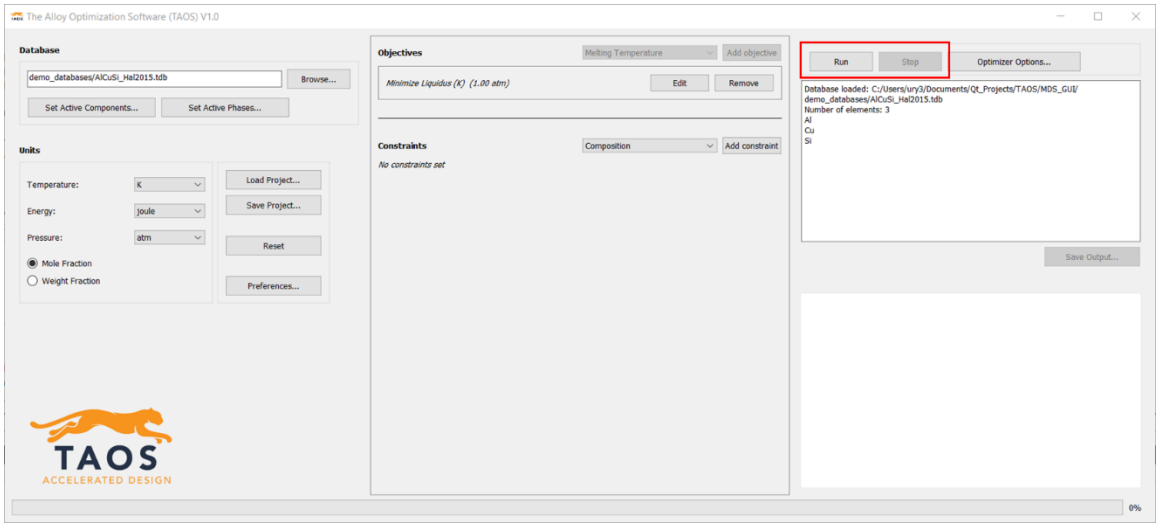


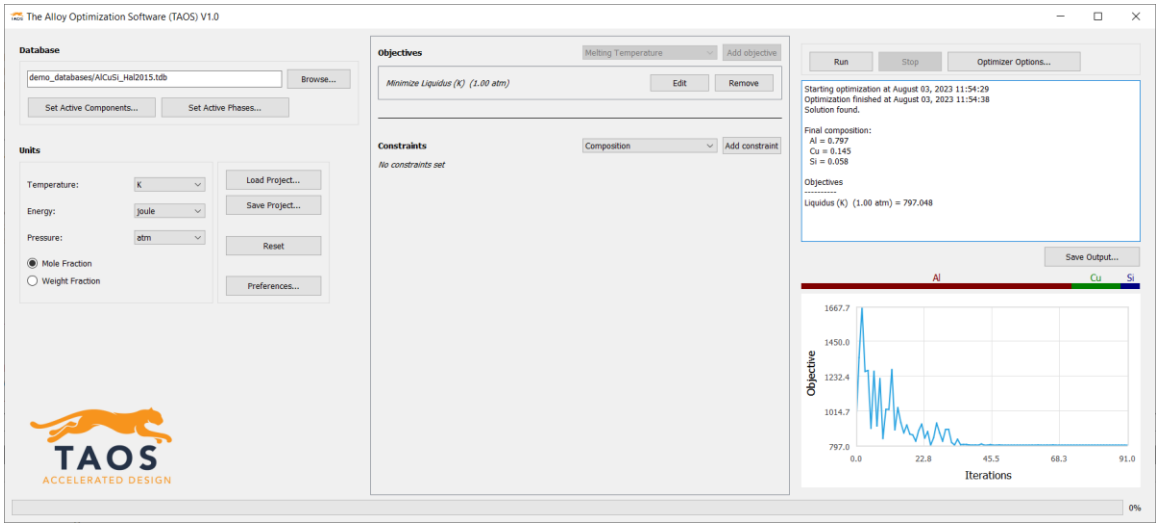
3. In the “Objectives” section, select “Melting Temperature” and click add Objective. A small window should show up. Since we want to minimize the liquidus temperature, we do not have to change any parameters here. Click “OK” and the objective should show up in the main window.





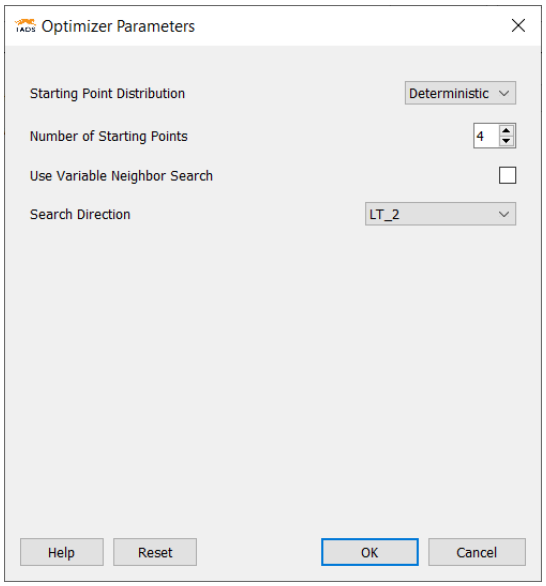
4. Now that the problem is valid, click “Run” to start the optimization. The results should converge at 797 K at $Al_{0.797}Cu_{0.145}Si_{0.058}$





‘

5. Some problems are more difficult to optimize than others as they could be highly constrained or have many local optima. You can have some control over the optimizer parameters by clicking on “Optimizer Options…” (see 8.5.3). Note: Variable neighbor search may be used to problems with many local optima.

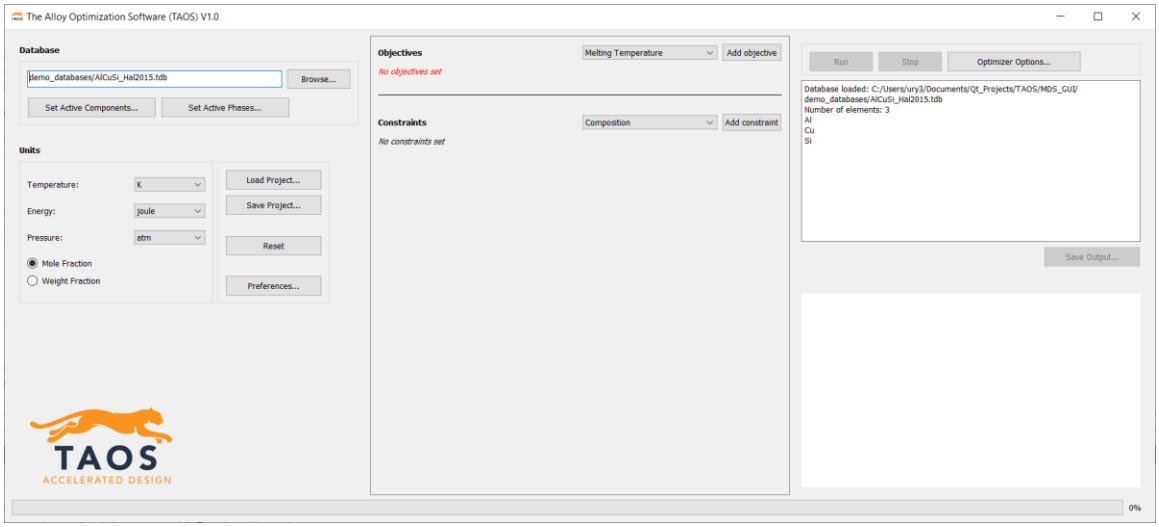


7.2. Example – Constrained Optimization (Al-Cu-Si)

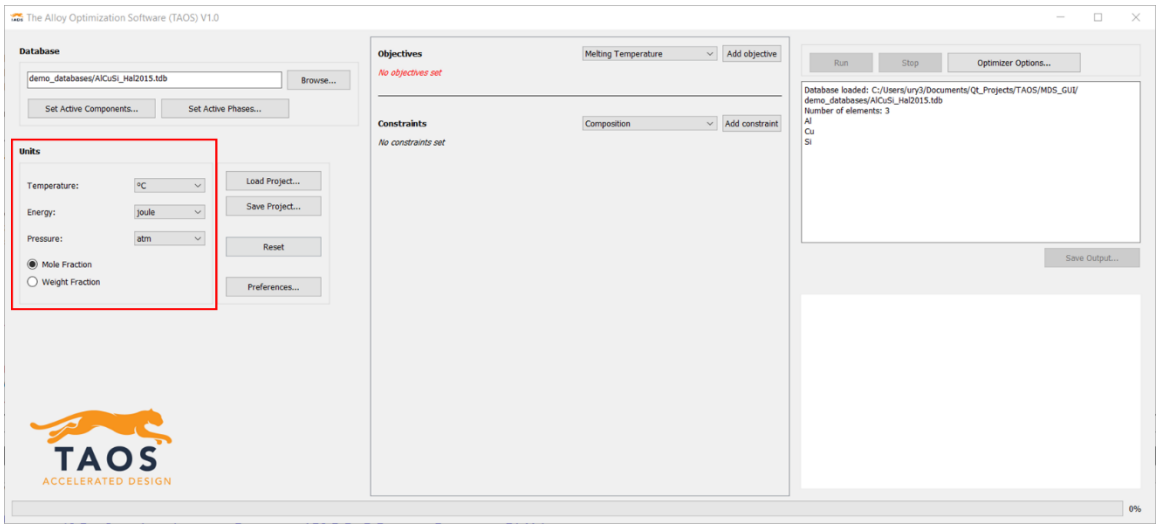
Problem: $minimize \quad Solidification\ range$

$subject\ to \quad Al_2Cu \geq 0.3\ at\ 500°C$
$\beta\text{-}Si\ (\text{Diamond\_A4}) \geq 0.05\ at\ 500°C$

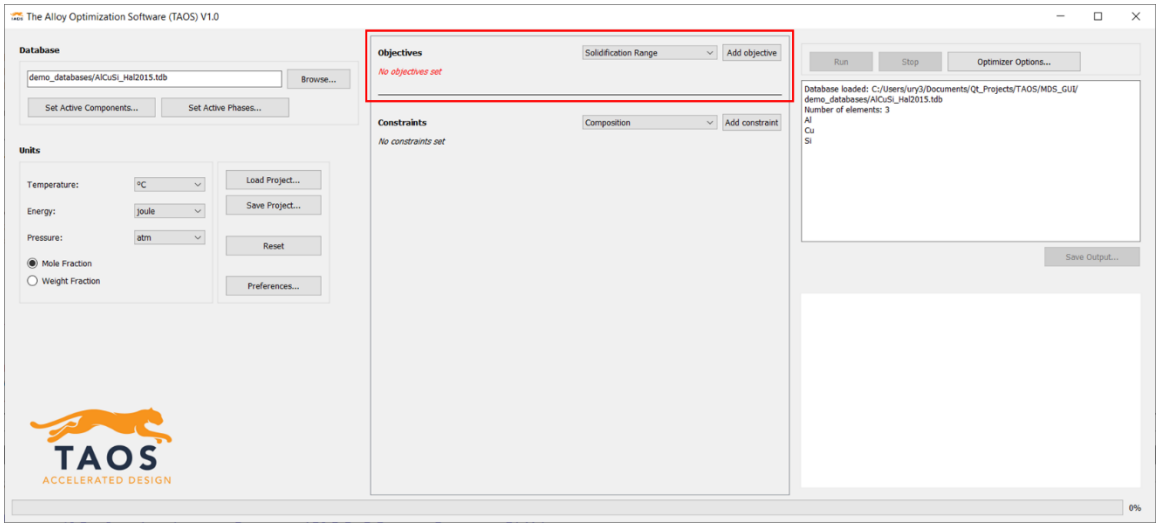
1. Load the AlCuSi_Hal2015.tdb database.

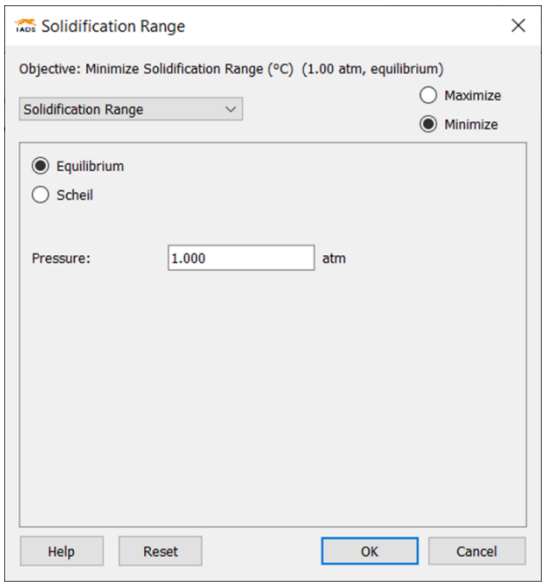


2. In the “Units” window, change the Temperature units to “°C”.

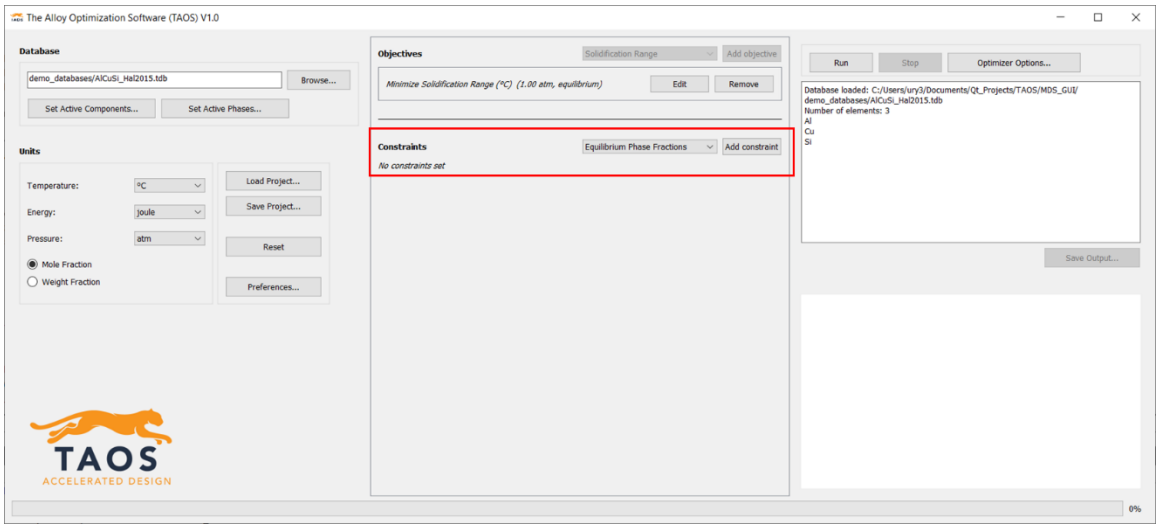


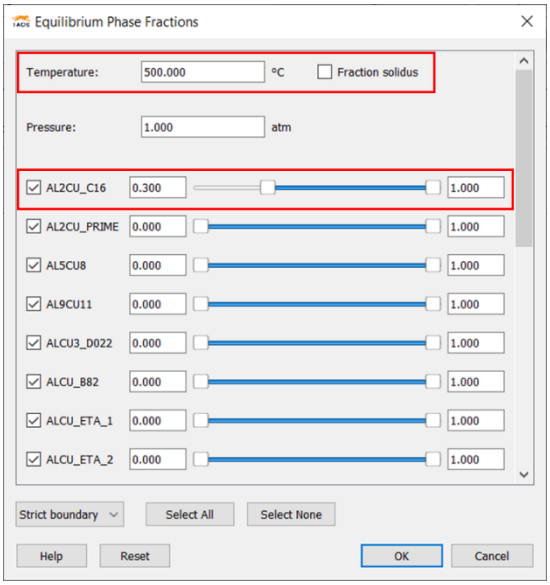
3. In the “Objectives” section, change the selection to “Solidification Range” and click “Add Objective”. Here, we want to minimize the solidification range determined by the equilibrium liquidus and solidus, so we can leave the parameters the same here.

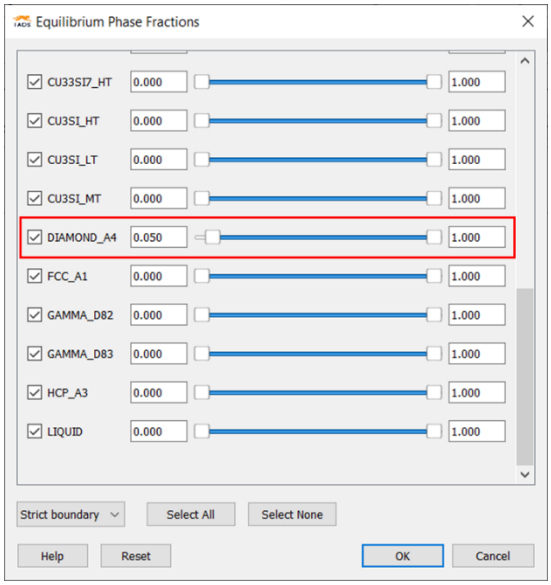




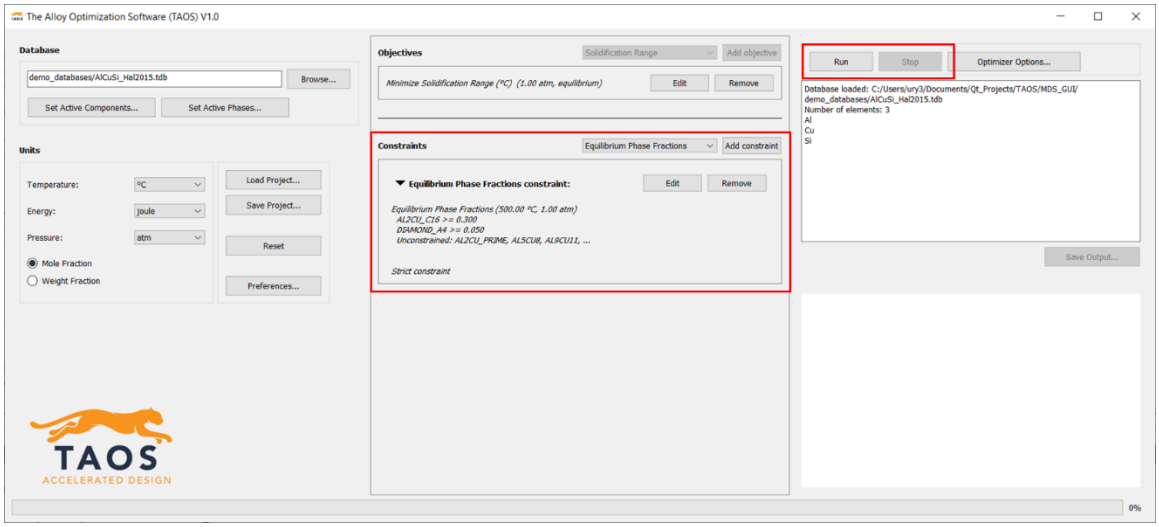
4. In the “Constraints” section, change the section to “Equilibrium Phase Fractions” and click “Add Constraint”. You should be prompted with another window.
    a. Since we want to constraint the Al_2Cu and β-Si phase fractions to a minimum value, drag the sliders or change the value in the lower bound to 0.3 for AL2CU_C16 and 0.05 for DIAMOND_A4. Set the temperature to 500°C.
    b. Click “OK” to set the constraint. You can show the constraint summary by clicking on the title of the title of the new constraint “Equilibrium Phase Fraction Constraint:”

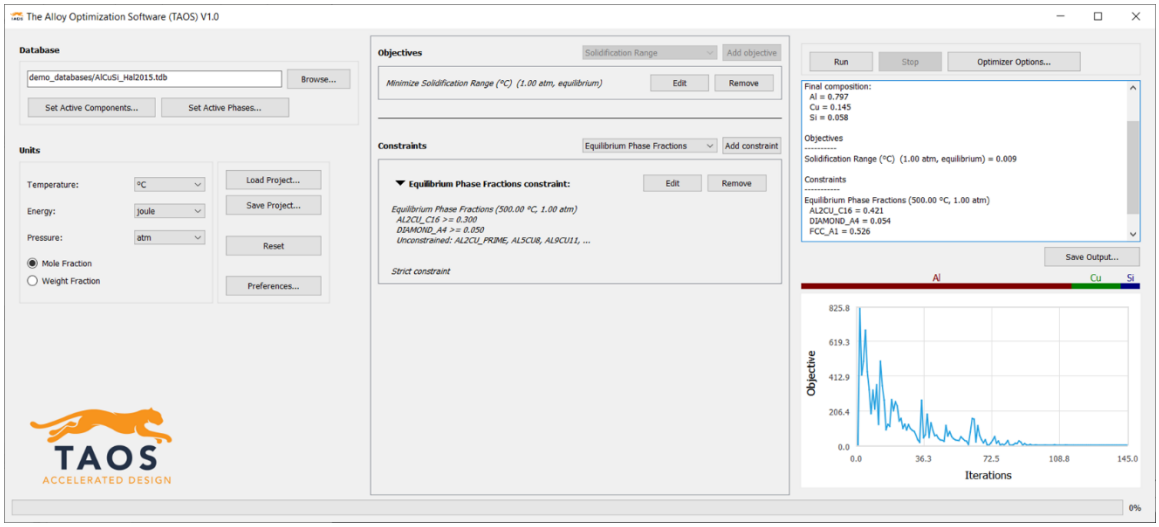






5. The problem is now set up to run. Click “Run” to start the optimization. The final composition should be $Al_{0.797}Cu_{0.145}Si_{0.058}$. The results may vary a little bit due to local minima in this problem.



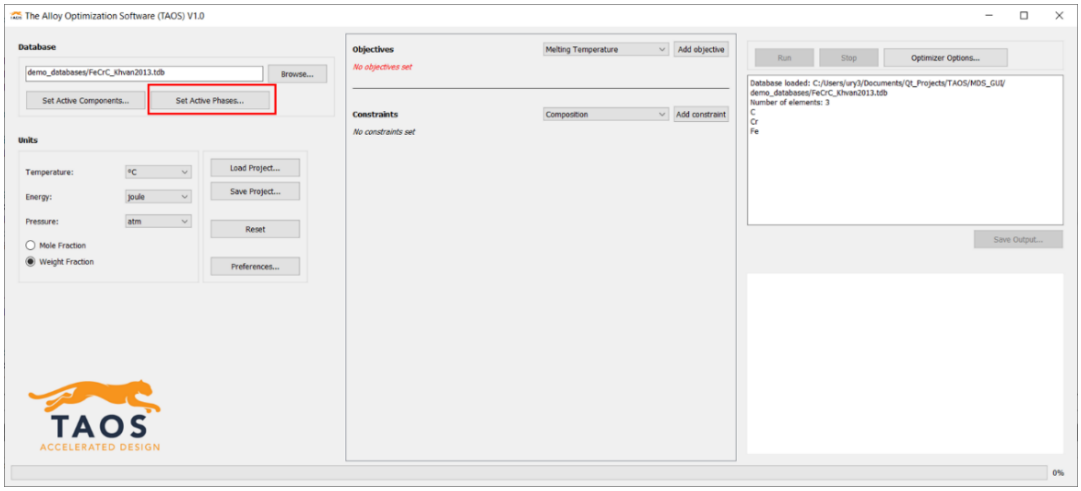


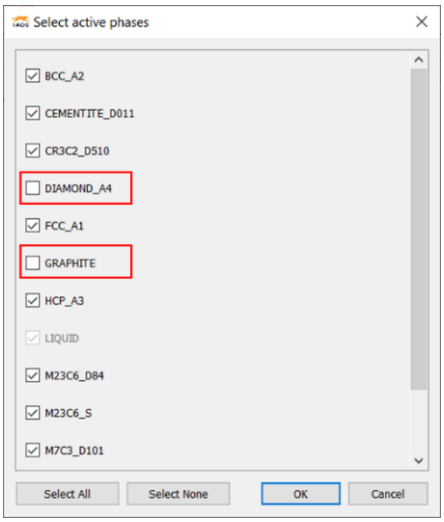
7.3. Example – Suspending Active Phases during Optimization (Fe-Cr-C)

$$\text{Problem:} \quad \textit{maximize} \quad M_{23}C_6 + M_7C_3 \; at \; 600°C$$

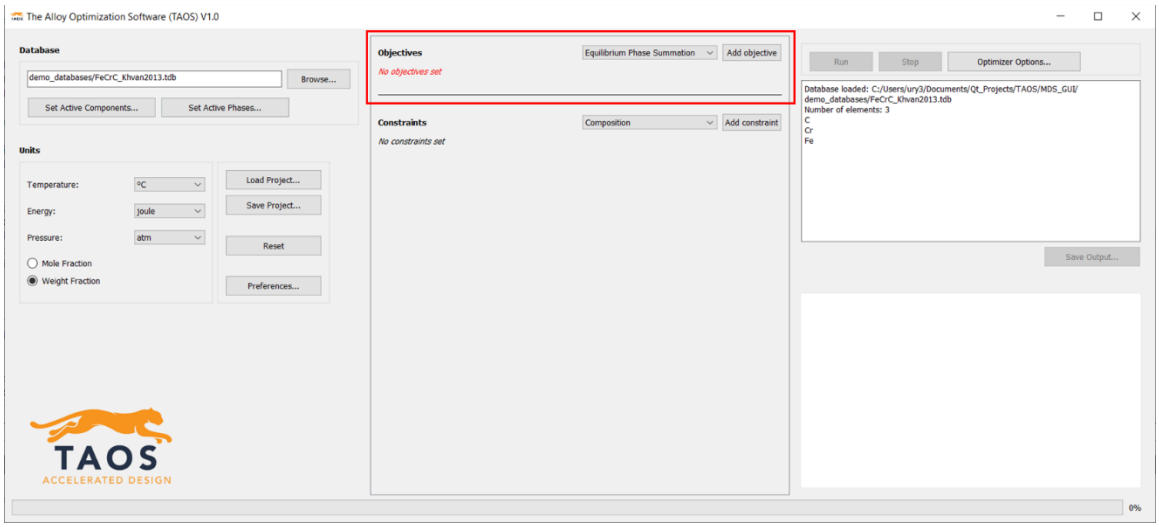
$$\textit{subject to} \quad w(C) \leq 0.06$$
$$w(Fe) \geq 0.8$$
$$BCC\_A2 \geq 0.8 \; at \; 600°C$$
$$Only \; FCC\_A1 \; at \; solidus$$

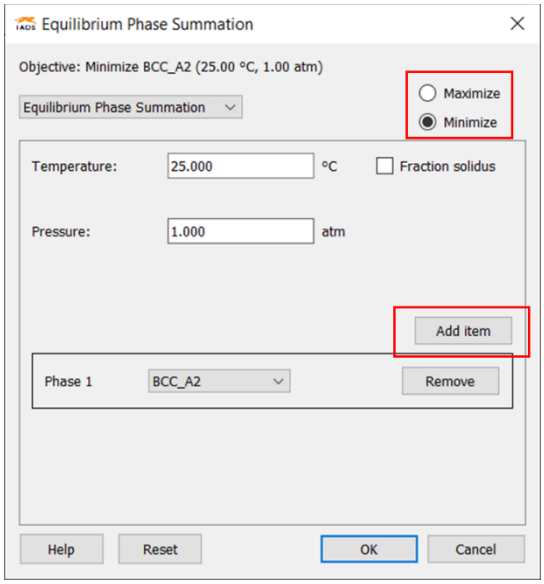
1. Load the FeCrC_Khvan2013.tdb data and change the temperature units to °C and the composition units to weight fraction.
2. In the Fe-Cr-C system, carbides are metastable due to the high stability of graphite. However, the formation of graphite slow enough that carbides are observed experimentally. To account for this, we need to suspend graphite and diamond from the equilibrium calculations (diamond is also suspended here also due to its high stability and slow kinetics). Click on "Select Active Phases…". This will bring up a window with all the phases in the database. Uncheck GRAPHITE and DIAMOND_A4.

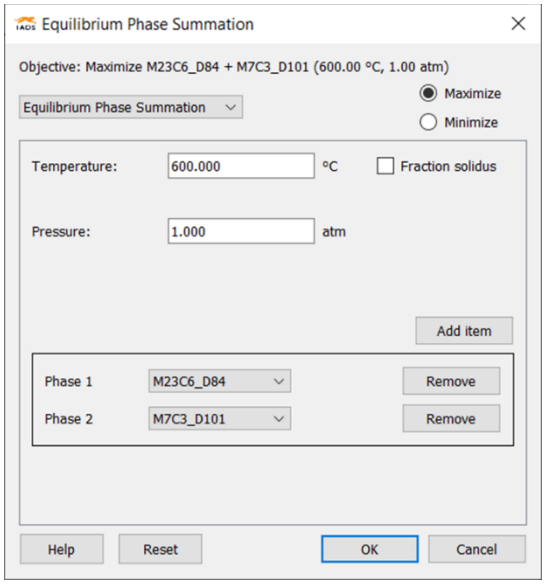




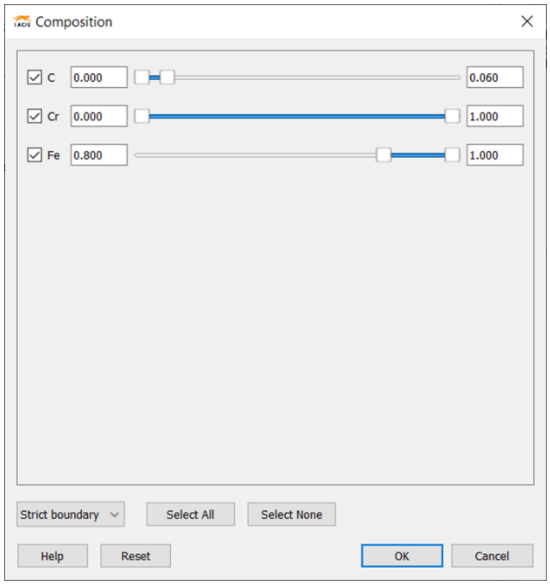
3. In the “Objectives” section, select “Equilibrium Phase Summation” and click “Add Objective”. Unlike the previous examples, we will need to set some of the parameters here. Change the temperature to 600°C. To set the phases, click on “Add item” to add a second phase. Then select M23C6_D84 and M7C3_D101 for phase 1 and 2. Since we want to maximize this value, click the “Maximize” button.



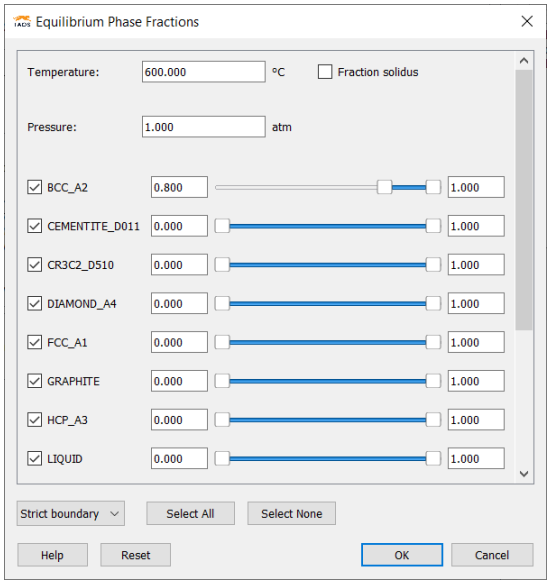




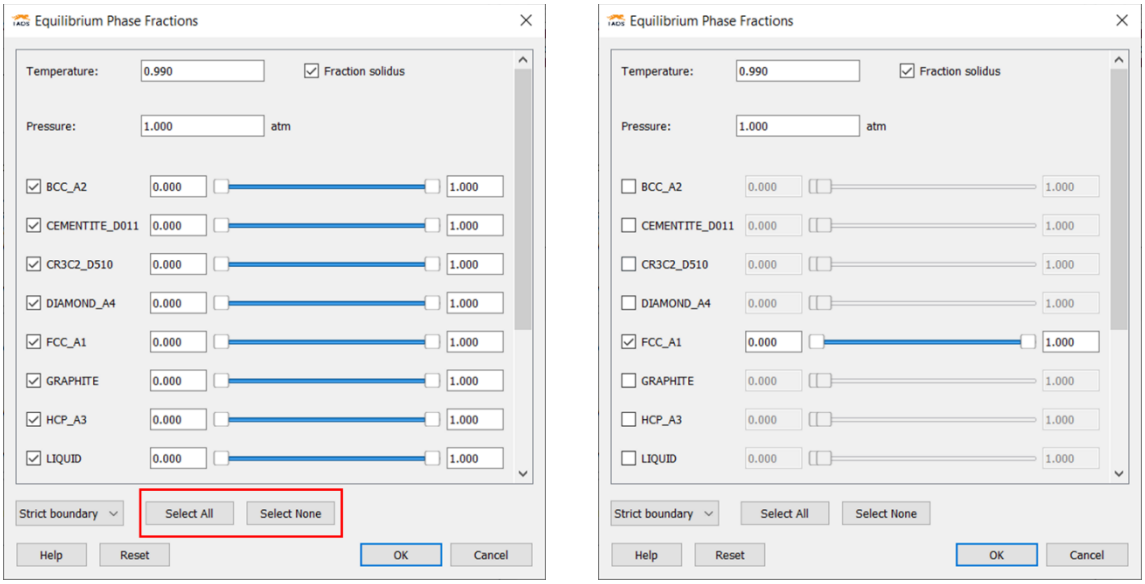
4. In the “Constraints” section, select “Composition” and click “Add Constraint”. Adjust the C range to [0.000, 0.060] and the Fe range to [0.800, 1.000].



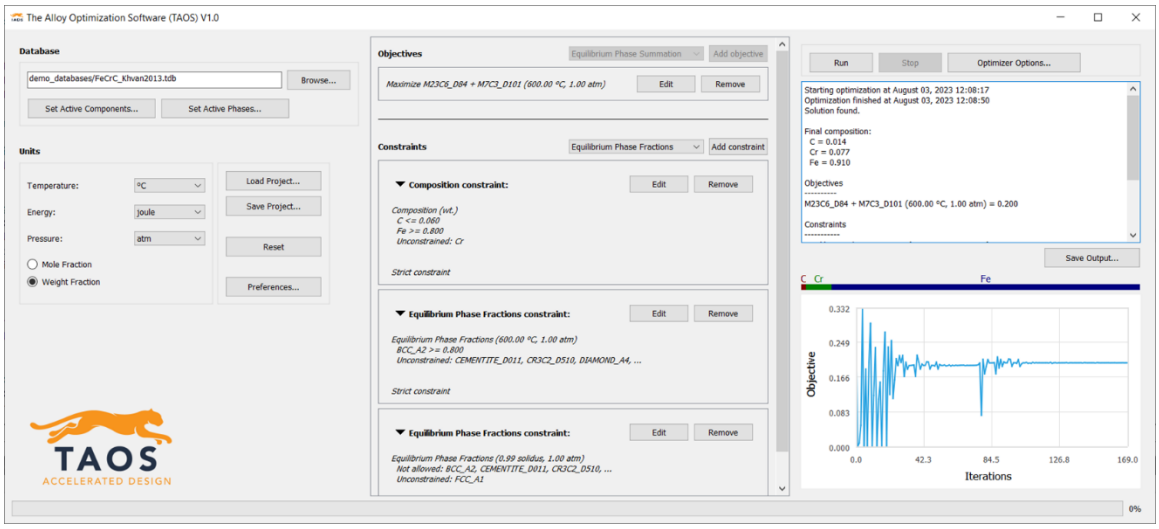
5. Select “Equilibrium Phase Fractions” in the “Constraints” section and click “Add Constraint”. In this window, change the temperature to 600°C and set the BCC_A2 range to [0.800, 1.000].



6. Add another “Equilibrium Phase Fractions” constraint. For this constraint, set the temperature to 0.99. Any value below 1 will tell the optimizer to calculate equilibrium at a fraction of the equilibrium solidus. In this case, this will calculate at 0.99 of the solidus. To restrict all phases from forming except for FCC_A1, click the “Select None” button to uncheck all the phases. Then check FCC_A1. This will leave FCC_A1 unconstrained while constraining all the other phases to not be stable at equilibrium.



7. Click “Run” to start the optimization. This is a problem where the solution is a region of compositions. At the solution, the objective and the M_7C_3 fraction at 600°C should be 0.2.

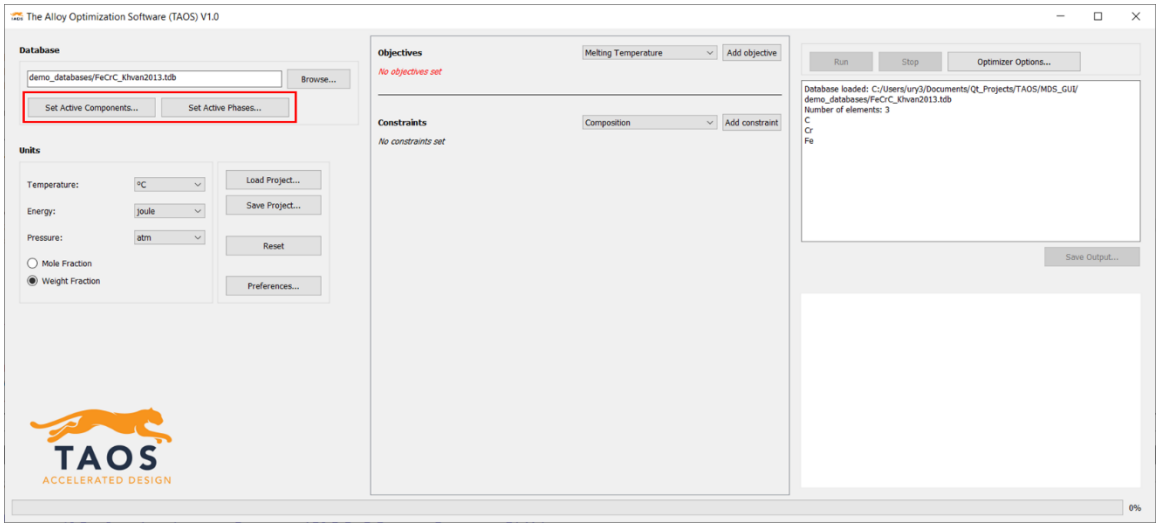


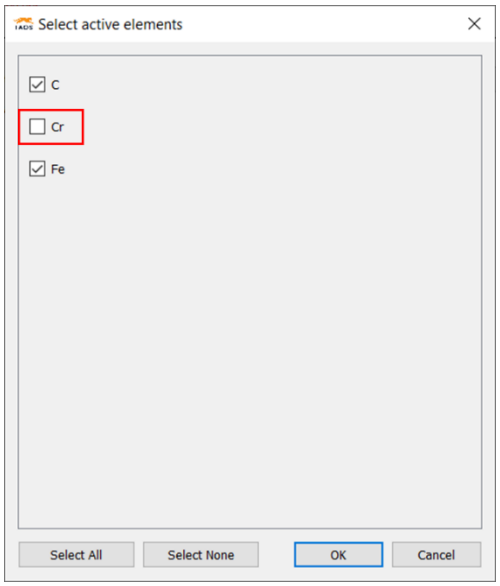
7.4 Example – Suspending Active Components (Fe-Cr-C)

Problem: $minimize \quad Solidification\ range$

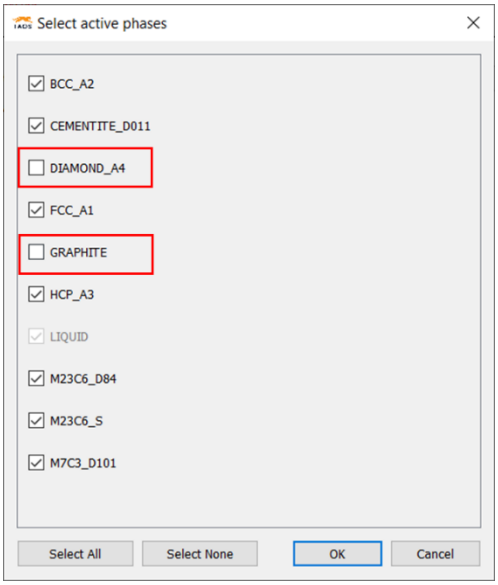
$subject\ to \quad w(C) \leq 0.02$
$0.025 \leq Fe_3C \leq 0.1\ at\ 750°C$
$Only\ FCC\_A1\ at\ 950°C$
$Only\ FCC\_A1\ at\ solidus$

1. Load the FeCrC_Khvan2013.tdb database. Set the temperature units to °C and composition units to weight fraction.
2. Since we only care about Fe and C, we want to remove Cr from the system. Click on "Set Active Components…". This will show all the components in the database. Uncheck Cr. This will update the thermodynamic system and the possible phases to ones that can form with only Fe and C.

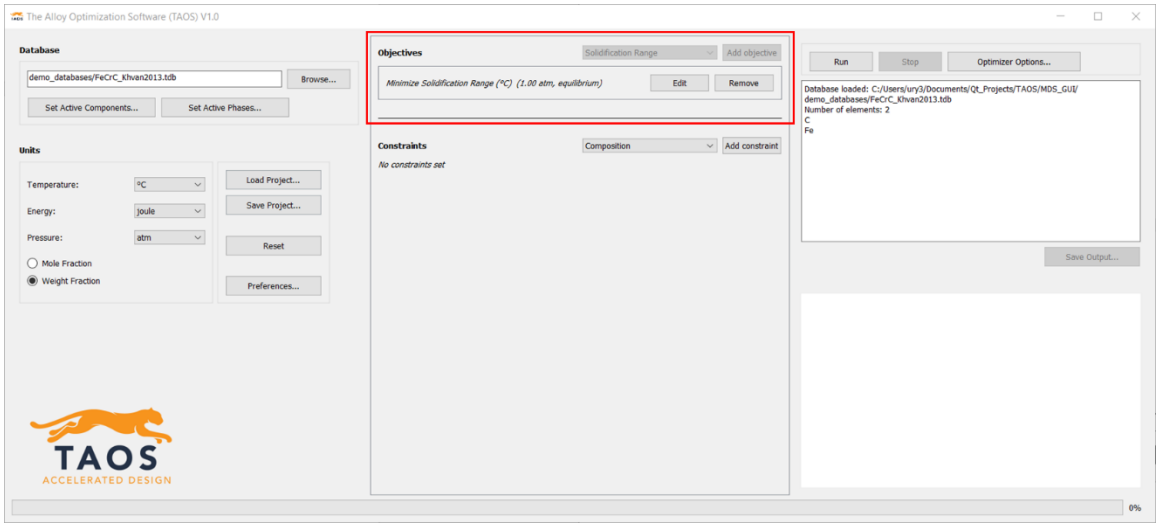




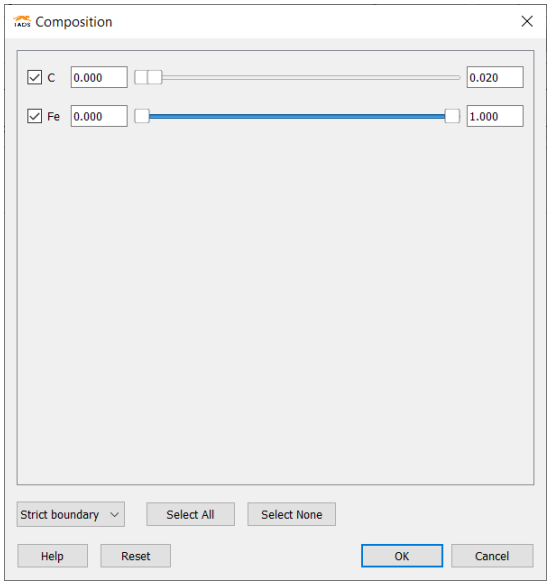
3. Click on “Set Active Phases…” and uncheck GRAPHITE and DIAMOND_A4.



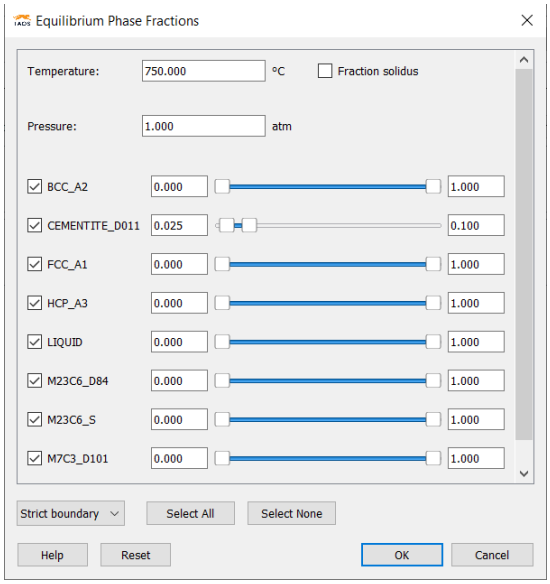
4. In the “Objectives” section, set the objective to minimize solidification range.



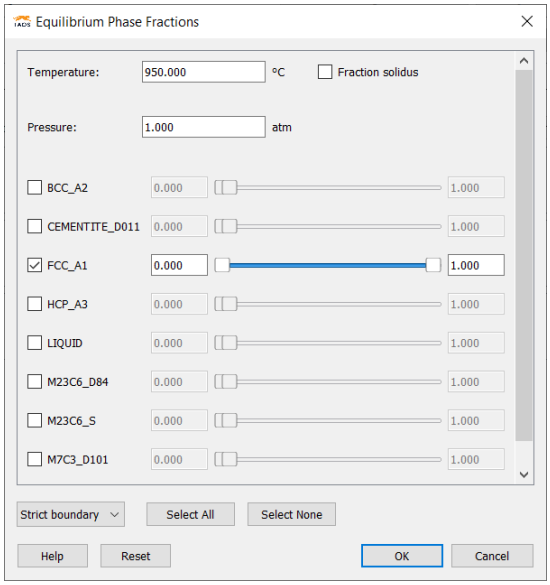
5. Add a “Composition” constraint and set the C range to [0.000, 0.020].



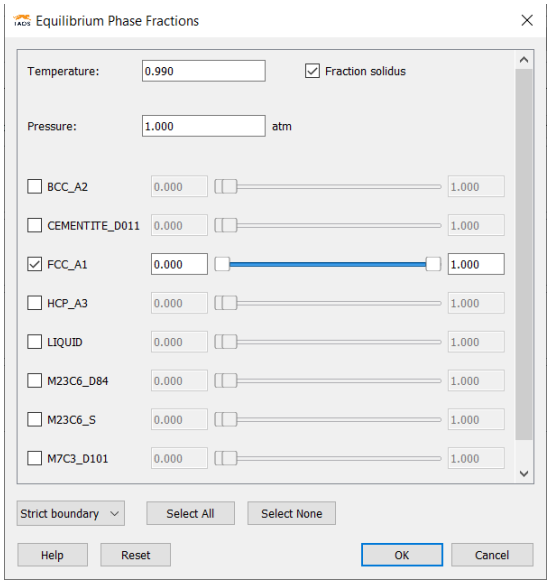
6. Add an “Equilibrium Phase Fraction” constraint and set the temperature 750°C. Set the CEMENTITE_D011 range to [0.025, 0.100].



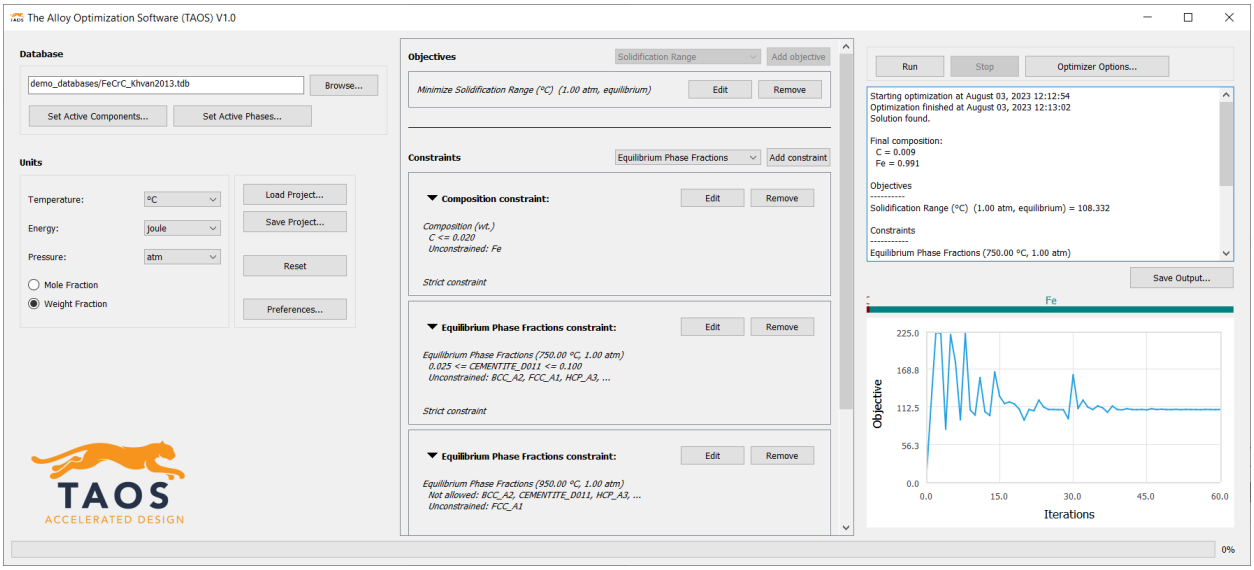
7. Add another “Equilibrium Phase Fraction” constraint and set the temperature to 900°C. Uncheck all phases except for FCC_A1.



8. Repeat step 7, but with the temperature at 0.99 of the solidus temperature.



9. Click “Run” to start the optimization. The final composition should be $C_{0.009}Fe_{0.991}$

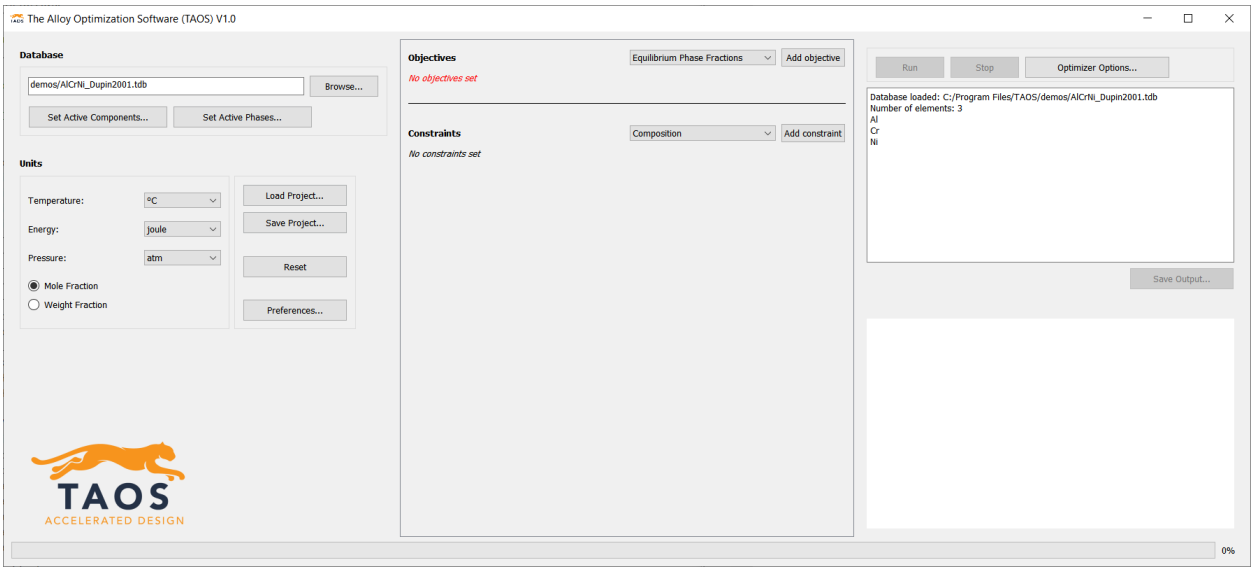


7.5. Example – Ordered and Disordered Phase Models (Al-Cr-Ni)

Problem: $maximize \quad FCC\_L12 \; at \; 750^oC$

$subject \; to \quad x(Cr) \geq 0.1$
$x(Ni) \geq 0.5$
$FCC\_A1 \geq 0.05 \; at \; 750^oC$
$FCC\_L12 \geq 0.10 \; at \; 750^oC$
$FCC\_A1 + FCC\_L12 = 1 \; at \; 750^oC$

1. Load the AlCrNi_Dupin2001.tdb database from the database folder and set the temperature units to °C.



2. In this system, the FCC and BCC phases can exhibit long-range ordering (L12 and B2, respectively) over a range of temperatures and compositions. In the AlCrNi_Dupin2001.tdb database, the ordered and disordered states of these phases are modeled as a single Gibbs free energy curve using the partitioned model. When this model is used, TAOS calculates the degree of ordering for each phase to allow for optimization problems to have an objective or constraint applied on the ordered or disordered state of the phase.

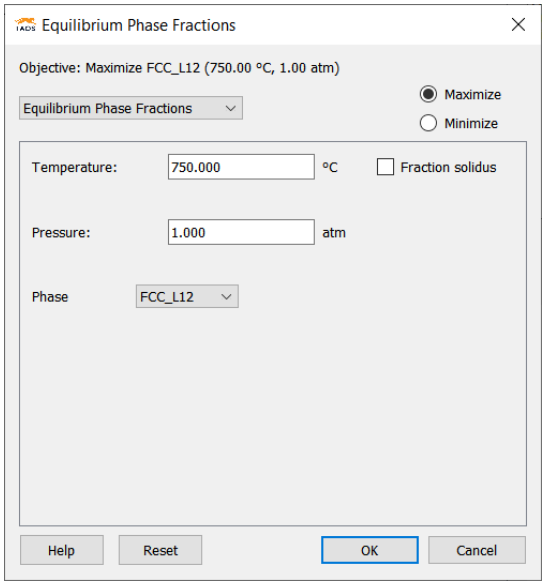
    a. Due to differences between PyCalphad and Thermo-Calc thermodynamic engines, the names of the ordered and disordered phases will be the following:

Thermodynamic Software	Sum of disordered phases	Sum of ordered phases
PyCalphad	FCC_A1, BCC_A2	FCC_L12, BCC_B2
Thermo-Calc	FCC_L12, BCC_B2	FCC_L12#2, BCC_B2#2

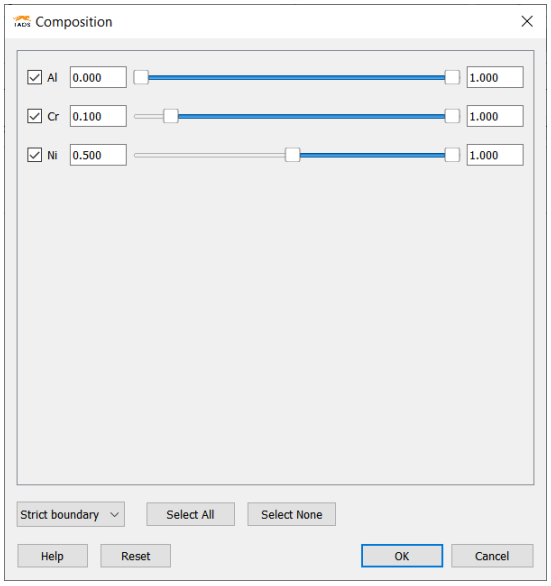
    b. Note that in the presence of multiple disordered and/or ordered phases (e.g., FCC_A1 miscibility gap), their phase fractions are added and reported in the corresponding disordered and/or ordered phases (e.g, FCC_A1).

c. The examples will use the naming conventions defined for PyCalphad. If the problem is being set up using TC-Python, make sure that the corresponding phase names are used instead (replace FCC_Al with FCC_L12 and FCC_L12 with FCC_L12#2).

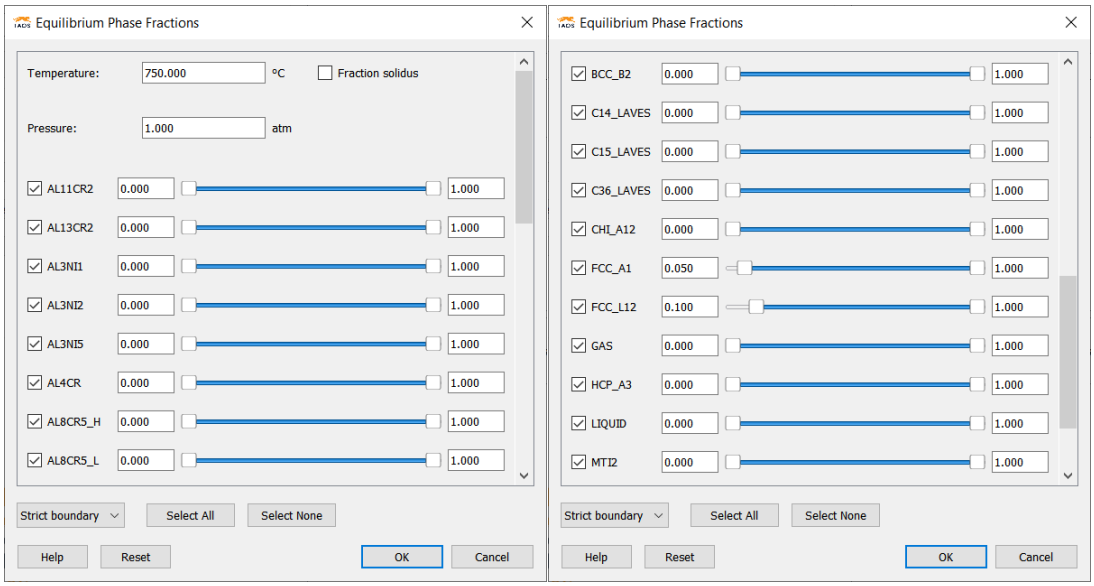
3. Set the objective to maximize the amount of FCC_L12 at 750 °C using the Equilibrium Phase Fraction objective.



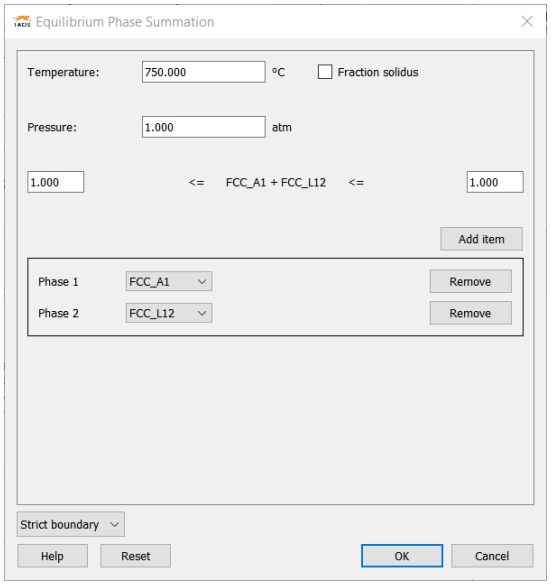
4. Add a Composition constraint. Set the Cr range to [0.100, 1.000] and Ni range to [0.500, 1.000]



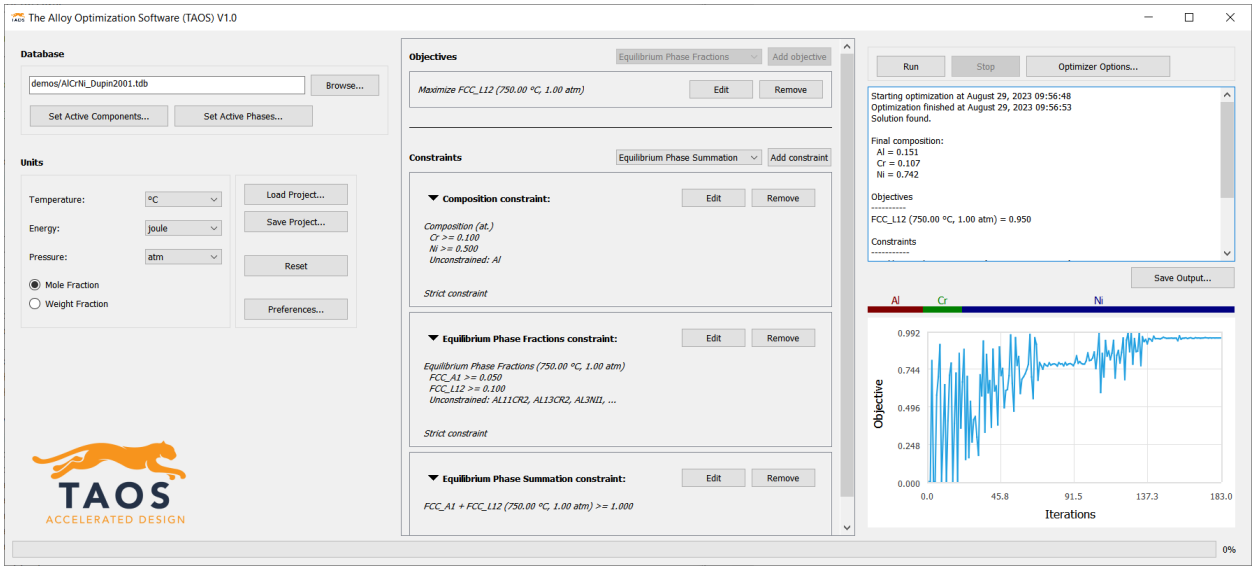
5. Add an Equilibrium Phase Fraction constraint and set the FCC_A1 range to [0.050, 1.000] and FCC_L12 range to [0.100, 1.000] at 750 °C.



6. Add an Equilibrium Phase Summation constraint and set it to limit the sum of FCC_A1 and FCC_L12 to 1 (set the range to [1.000, 1.000]) at 750 °C. This will treat the formation of any other phases as a violation of this constraint.



7. Click “Run” to start the optimization. The solution exists over a region of compositions, but at the solution, the amount of FCC_L12 at 750 °C will be 0.95 (the maximum amount given the Equilibrium Phase Fraction constraint).
    a. There are several local minima that the optimizer can get stuck on in this problem. This can be resolved by running the optimizer several times or changing some of the parameters in the Optimizer Options. Increasing the number of starting points or enabling VNS will increase the likelihood of finding the global minimum.



8. Documentation

8.1. Database Selection and System Definition

8.1.1. Browse

- Opens a file browser to load a thermodynamic database compatible with the current active thermodynamic software.

Thermodynamic Software	Compatible Database Formats
PyCalphad	TDB, DAT
Thermo-Calc (through TC-Python)	TDB DB (Full version only)

- Note: The demo version limits database selection to the following: AlCrNi_Dupin2001.tdb, AlCuSi_Hal2015.tdb and FeCrC_Khvan2013.tdb (these are included in the TAOS distribution in the "demos" folder).

8.1.2. Set Active Components

- Brings up a dialog to select or deselect active components in the database. This will cause the software to only load phases that can form with the selected components.
- Select All: Selects all components.
- Select None: deselects all components. Note: at least 2 components must be active to set up an optimization problem.
- Note: Changing the list of active components will reset the optimization problem definition as it changes the set of available phases.

8.1.3. Set Active Phases

- Brings up a dialog to select or deselect active phases in the database. This is generally not recommended unless there are good reasons to disable a phase from equilibrium (see Examples 7.3 and 7.4).
- Select All: Selects all phases.
- Select None: deselects all phases. Note: at least 2 phases must be active to set up an optimization problem.
- Note: If a liquid phase is detected in the database, it will not be allowed to be disabled.

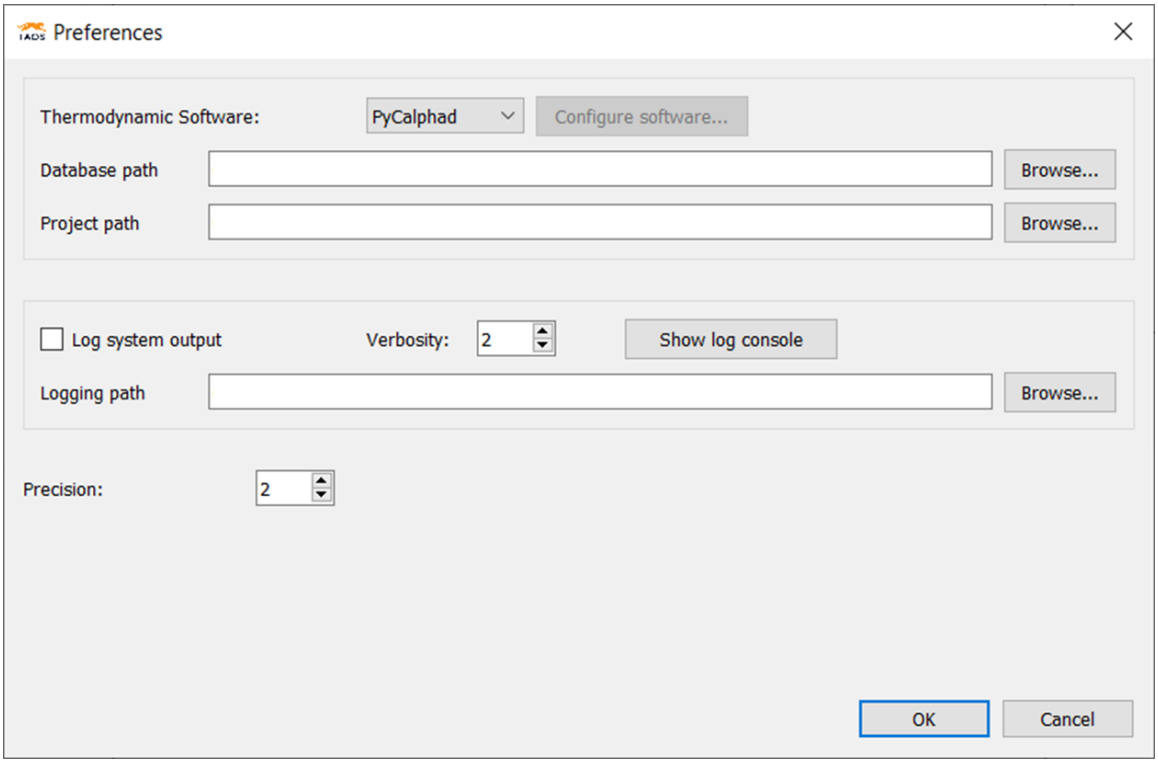
8.2. Units

TAOS supports both SI and Imperial units. The following available units are listed below with the default unit being bolded.

- Temperature: °C, **K**, °F.
- Energy: **joule**, cal (kCal)
- Pressure: Pa, **atm**, bar, kbar, psi, torr
- Composition: **Mole fraction**, Weight fraction

8.3. Preferences

- Thermodynamic Software – selected software used for thermodynamic calculations.
    - Configure software – for software other than PyCalphad, this will try to find the path to the selected thermodynamic software and set up any necessary data to run the software.
- Database Path – initial search path for databases. Note: upon loading a database, the current search path will be updated to the last path the database was in.
- Project Path – initial search path for projects. Note: upon loading a project, the current search path will be updated to the last path the project was in.
- Logging Path – path to store log files.
- Log system output – whether to keep the current log file upon closing TAOS.
    - Note: a last session log file will always be recorded in case of software crashes.
- Verbosity – verbosity of the logging.
    - 0 – No log output
    - 1 – Minimal log output, will only show errors and minimal optimizer display
    - 2 (default) – will show errors, minimal optimizer display and calculation breakpoints in thermodynamic calculations
    - 3 – All log output – will show errors, all optimizer display and calculation breakpoints in thermodynamic calculations
- Show log console
    - Opens a dialog that will show the log output.
- Precision
    - Number of significant figures for composition and phase fractions.



8.4. Problem Setup

8.4.1. Load Project: Opens a file browser to load a project (.taos) file.

8.4.2. Save Project: Opens a file browser to save a project (.taos) file.

8.4.3. Reset

- Resets the problem definition.
- Note: this only resets the defined objective and constraints. This does not reset the system definition (i.e., active components and phases). Any changes to the list of active components and phases will be retained.

8.4.4. Objectives

- Add objective: Adds the current selected objective property and brings up a dialog to edit options.
- Edit: Brings up a dialog to edit the selected objective.
- Remove: Removes the selected objective.
- Objective dialog:
    - Minimize/Maximize
    - Help: Brings up help dialog for more information.
- Reset: Resets objective options to default values.

8.4.5. Constraints

- Add constraint: Adds the current selected constraint property and brings up a dialog to edit options.
- Edit: Brings up a dialog to edit the selected constraint.
- Remove: Removes the selected constraint.
- Constraint dialog:
    - Strict/Soft boundary: Sets constraint as a hard or soft boundary in the optimizer. Violation of strict boundary constraints will result in a failed black box evaluation. Soft boundary constraints can be violated, but the optimizer will try to relax the constraints so that the final solution does not violate them.
    - Help: Brings up help dialog for more information.
    - Reset: Resets constraint options to default values.

8.4.6. Properties

Most properties used as objectives or constraints will require a few additional settings to configure. Common settings include:

- Temperature – temperature at which to perform equilibrium calculations. If the temperature is less than 1, then it will be treated as a fraction of the equilibrium solidus.
- Pressure – pressure at which to perform equilibrium calculations. Note: many databases do not have support for pressure dependence. For these cases, changing the pressure will not affect the calculations.
- Equilibrium/Scheil – whether to assume equilibrium or Scheil assumptions during solidification.
    - Equilibrium - Infinitely fast diffusion in solid and liquid phases
    - Scheil – Infinitely fast diffusion in liquid but no diffusion in solid (see G.H. Gulliver, *J. Inst. Met.* 9 (1913) 120–157 and Scheil, *Zeitschrift Für Met.* 34 (1942) 70–72.)
    - For solidus calculation, using the Scheil assumption will return the temperature where the last liquid solidifies.
        - For solidification range, using the Scheil assumption will return the difference between the liquidus and the Scheil solidus.
    - For solidification phase fractions calculation, the equilibrium assumption will return the amount of each phase at equilibrium at the equilibrium solidus. The Scheil assumption will return the cumulative amounts of each phase that formed during a Scheil solidification simulation.

The following properties are available:

- Composition
    - As an Objective: Outputs the fraction of the current selection component
    - As a Constraint: Ranges set for each component will be used as the domain of the optimization problem. Unchecking a range will remove the component from the problem.
        - Select All: Selects all component ranges.
        - Select None: Deselects all component ranges. Note: At least 2 components must be enabled.

- Melting temperatures: Liquidus, Solidus (equilibrium), or Solidus (Scheil)

- Solidification range: Equilibrium or Scheil Solidification

- Solidification Phase Fractions
    - As an Objective: Outputs the fraction of the current selected phase at the solidus.
    - As a Constraint: Ranges define the minimum and maximum mole fraction for each phase at the solidus.
        - Unchecking a range will set a constraint for the phase fraction to be 0.

- Solidification Phase Summation
    - Similar to Solidification Phase Fractions but will output a single number representing the sum of 2 or more phases at the solidus.

- Equilibrium Phase Fractions
    - As an Objective: Outputs the fraction of the current selected phase at selected temperature.
    - As a Constraint: Ranges define the minimum and maximum mole fraction for each phase at selected temperature.
        - Unchecking a range will set a constraint for the phase fraction to be 0.

- Equilibrium Phase Summation
    - Similar to Equilibrium Phase Fractions but will output a single number representing the sum of 2 or more phases at selected temperature.

- Number of Elements
    - Outputs the number of elements with compositions above the defined threshold (mole or weight fraction).

- Composition Summation (Full version only)
    - Outputs a single number representing the sum of 2 or more elements.

- Growth Restriction Factor (Full version only)
    - Measure of how solute-limited diffusion affects solidification kinetics. A larger GRF should result in smaller grain sizes upon solidification.
    - See D. StJohn et al, "The contribution of constitutional supercooling to nucleation and grain formation" *Metallurgical and Materials Transactions A* 46 (2015) p. 4868-4885. https://doi.org/10.1007/s11661-015-2960-y

- Partition Coefficient (Full version only)
    - As an Objective: Outputs the partition coefficient ($C_{s,i}/C_{l,i}$) for the current selected component.
    - As a Constraint: Ranges define the minimum and maximum partition coefficient for each component.

- Cracking Index (Full version only)
    - Options:
        - Cracking susceptibility criterion (CSC)
        - Improved CSC (iCSC)
        - Kou's criterion
        - Simplifed Rappaz-Drezet-Gremaud model (sRDG)
        - See Z. Yang et al., "Design methodology for functionally graded materials: Framework for considering cracking" *Additive Manufacturing* 73 (2023) p. 103672. https://doi.org/10.1016/j.addma.2023.103672

8.5. Optimization

Optimization in TAOS is performed through the Nomad black box optimizer using the Mesh Adaptive Direct Search (MADS) algorithm. More information can be found here: https://www.gerad.ca/en/software/nomad/

8.5.1. Run: Starts the optimization problem.

8.5.2. Stop: Prematurely stops the optimization problem and uses the current best solution as the final composition.

8.5.3. Optimizer Options

- Starting point distribution
  - Deterministic
  - Random
- Number of starting points
  - Default: Number of active components + 1
- Use variable neighbor search: For problems with local optima, this will perform additional MADS runs in aim of finding the global optimum.
- Search direction: TAOS offers a few options from the available search directions implemented in Nomad. The main difference between LT and ORTHO is that LT will produce a set of random vectors as the basis for the search direction, while the basis vectors for ORTHO will be orthogonal. The number after LT or ORTHO denotes the number of directions that are generated during each poll step.
  - LT_2
  - LT_1
  - ORTHO_NP1_UNI
  - ORTHO_NP1_QUAD
  - ORTHO_2
  - ORTHO_2N
- More information about LT and ORTHO search directions can be found here:
  - LT search directions: C. Audet and J. Dennis, "Mesh adaptive direct search algorithms for constrained optimization" *SIAM Journal on Optimization* 17 (2006) p. 188-217. https://doi.org/10.1137/040603371
  - ORTHO search directions: M. Abramson et al, "OrthoMADS: A deterministic MADS instance with orthogonal directions" *SIAM Journal on Optimization* 20 (2009) p. 948-966 https://doi.org/10.1137/080716980
  - ORTHO QUAD search directions: C. Audet et al, "Reducing the number of function evaluations in mesh adaptive direct search algorithms" *SIAM Journal on Optimization* 24 (2014) p. 621-642. https://doi.org/10.1137/120895056

8.5.4. Display

- Three types of displays are used in TAOS:
- Text box: This will display the final result of the optimization, including the final composition, the objective values and the constraint values.
    - Note: The existence of a solution depends on the constraints and whether they are set as strict or soft constraints.
    - If all constraints are satisfied, then a solution is found.
    - If all strict constraints are satisfied, but any soft constraints are violated, then the best infeasible (minimum constraint violation) solution is returned.
    - If at least one strict constraint is not satisfied, then no solution is found.

8.5.5. Save Output

- Saves the result of the optimization into a text file (.txt). It will include the following information:
    - Database
    - Active Elements
    - Suspended Phases
    - Problem Definition
        - Objective
        - Composition limits
        - Constraints (all constraints will be shown, labeled as C0, C1, …)
    - Results:
        - Final composition
        - Values of the objective and constraints
    - Optimization History
        - Includes all the points that were evaluated as a table where the columns are elements, objectives, then constraints (Sum1 and Sum2 columns are here by default to constrain the overall alloy composition to be equal to unity, then listing constraints using the same labeling as in the problem definition of the file)