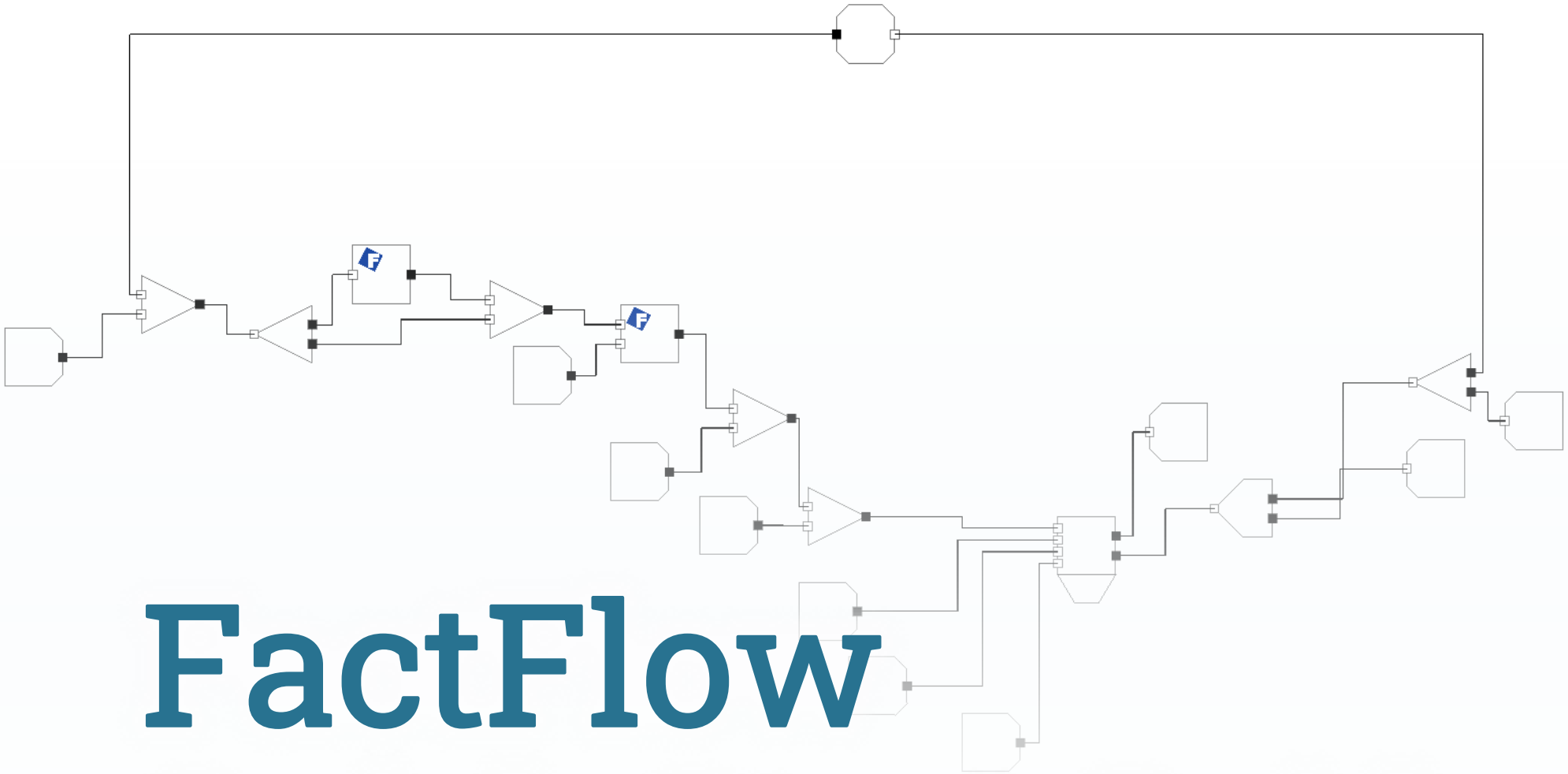
FactFlow



FactFlow Quick Start Guide

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What's "FactFlow" ?

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- Analysis
- Data Export
- Support

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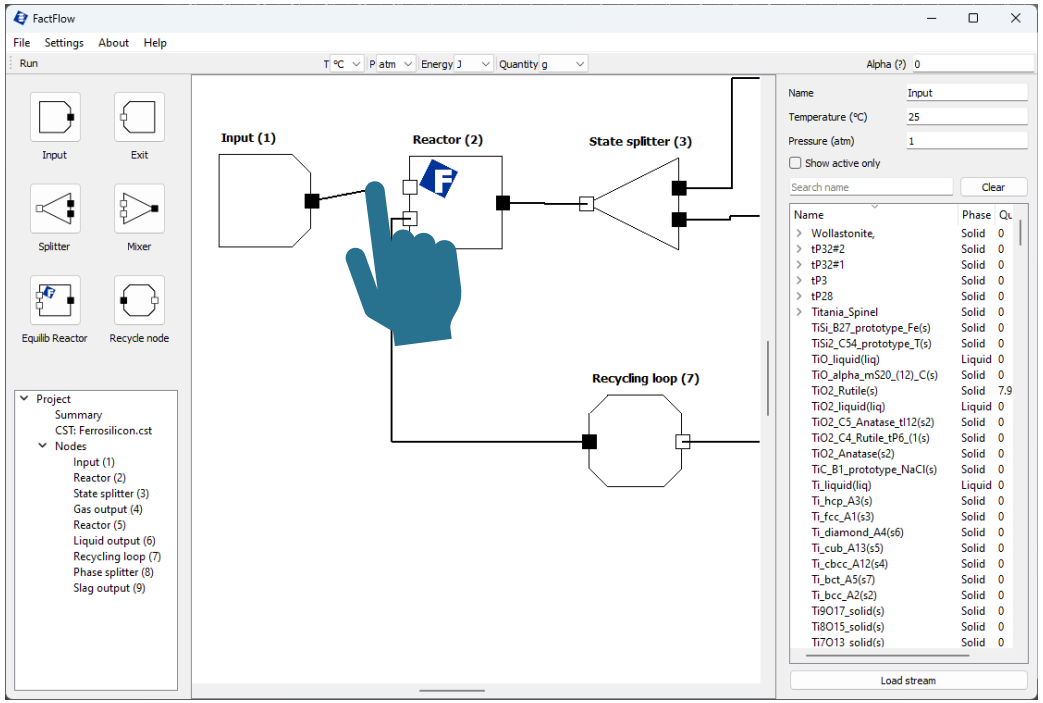
What is "FactFlow" ?



FactFlow stands as a cutting-edge tool designed for process simulation and optimization, harnessing the computational power of FactSage and ChemApp. Key features include:

- **Powered by FactSage and ChemApp**: FactFlow integrates the robust thermodynamic engines of FactSage and ChemApp, offering unparalleled accuracy in chemical and process simulations.
- **Intuitive User Interface**: Designed to be user-friendly, FactFlow facilitates easy interaction, allowing users to efficiently build, run, and analyze simulations.

What's "FactFlow" ?

Additional notable features of FactFlow include:

- **Flexible Simulation Capabilities**: FactFlow supports a wide range of process simulation activities, from equilibrium calculations to complex process optimizations, accommodating both steady-state and dynamic simulations.
- **Comprehensive Analysis Tools**: Equipped with extensive analysis and visualization tools, FactFlow enables in-depth examination of simulation outcomes, including phase distributions, chemical reactions, and performance metrics.
- **Modular Design for Easy Customization**: The software's modular structure allows users to easily add or modify components and reactions to tailor simulations to specific needs.
- **Continuous Development and Support**: FactFlow is backed by a dedicated development team, ensuring regular updates, feature enhancements, and user support.

FactFlow is not just a tool but a comprehensive platform designed to simplify and optimize the process simulation experience, making it an essential asset for researchers, engineers, and professionals in the chemical and process industries.

FactFlow

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System and Software Requirements

- **Operating System**: Must be a Windows PC, with Windows 10 or later version installed.
- **RAM**: Recommended to have 16 GB or higher for optimal performance.
- **FactSage Requirement**: FactSage 8.3 or a later version is mandatory, along with a valid license.

Install FactFlow

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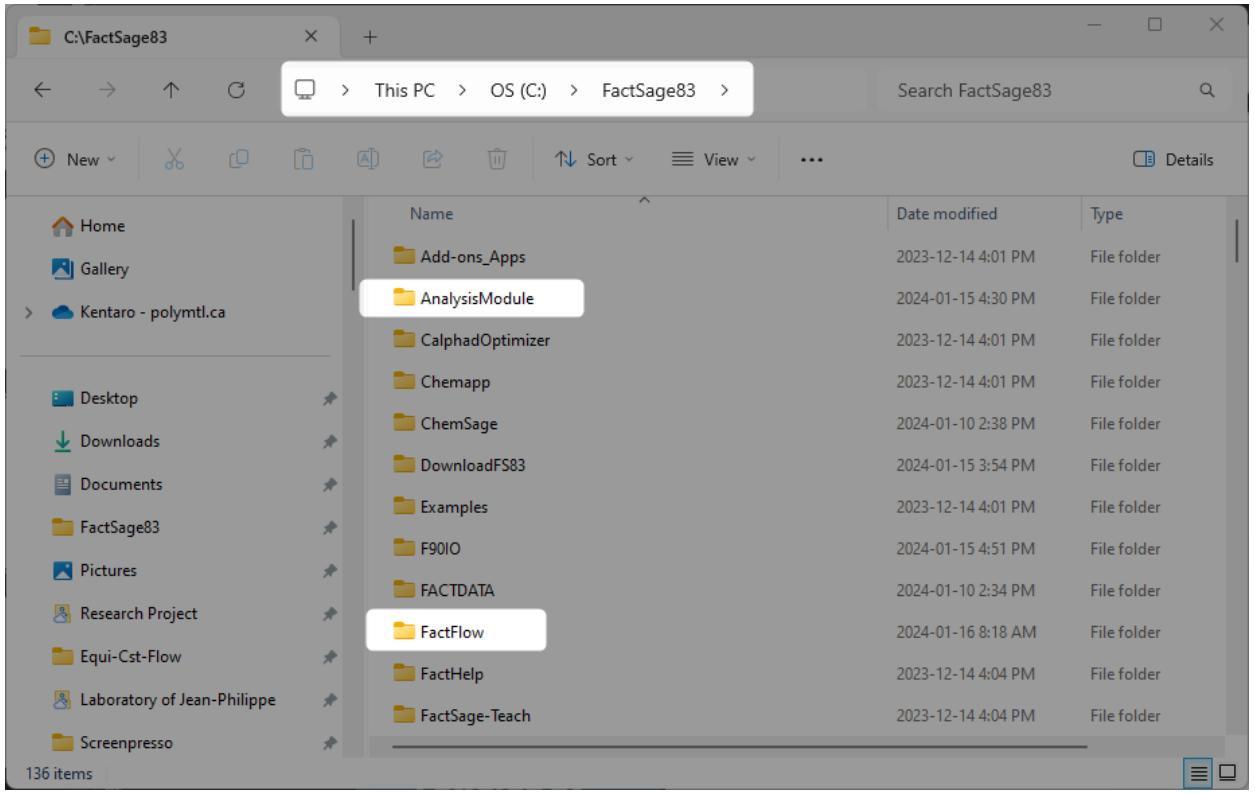
FactFlow Installation



1. **Download Files**: Save the provided zipped files for FactFlow and AnalysisModule.
2. **Unzip Files**: Unzip these files to get 'FactFlow' and 'AnalysisModule' folders.
3. **Open FactSage Folder**: Go to the FactSage root folder on your computer.
4. **Copy Folders**: Take both 'FactFlow' and 'AnalysisModule' folders.
5. **Paste in FactSage**: Place them directly into the FactSage root folder.

FactFlow

Generate .cst file

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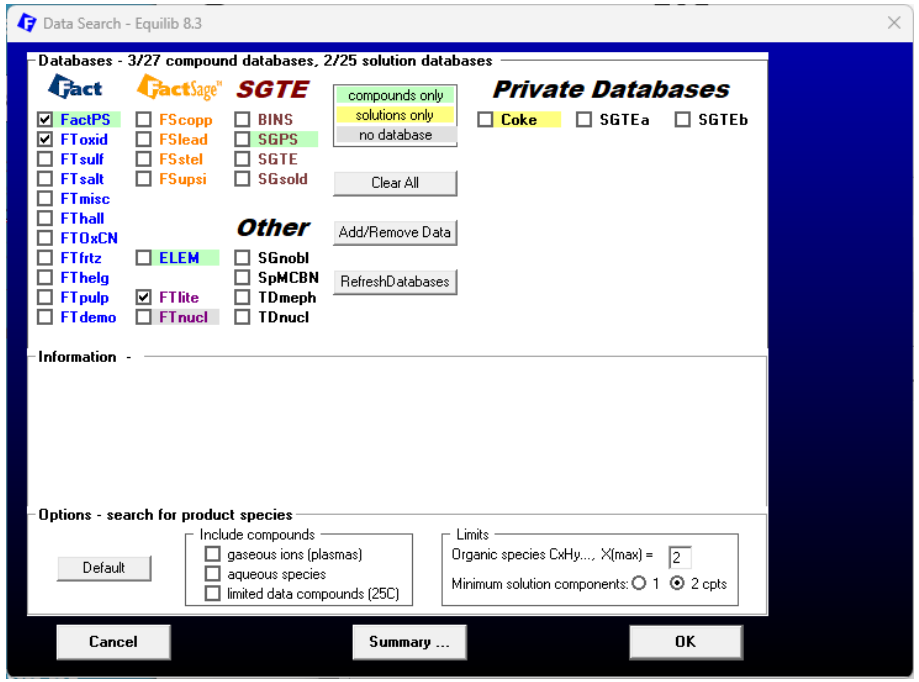
Generate .cst file



1. **Open Equilib Module: Start by opening the Equilib module.**
2. **Database Selection: Choose the appropriate Database for your simulation.**

FactFlow

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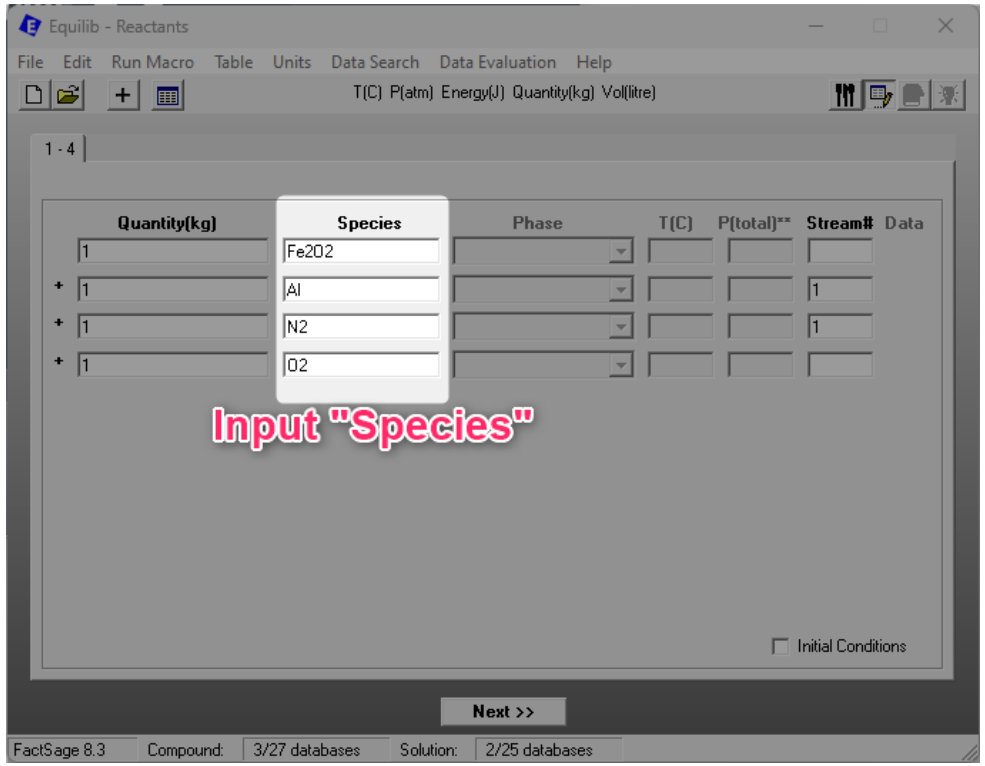
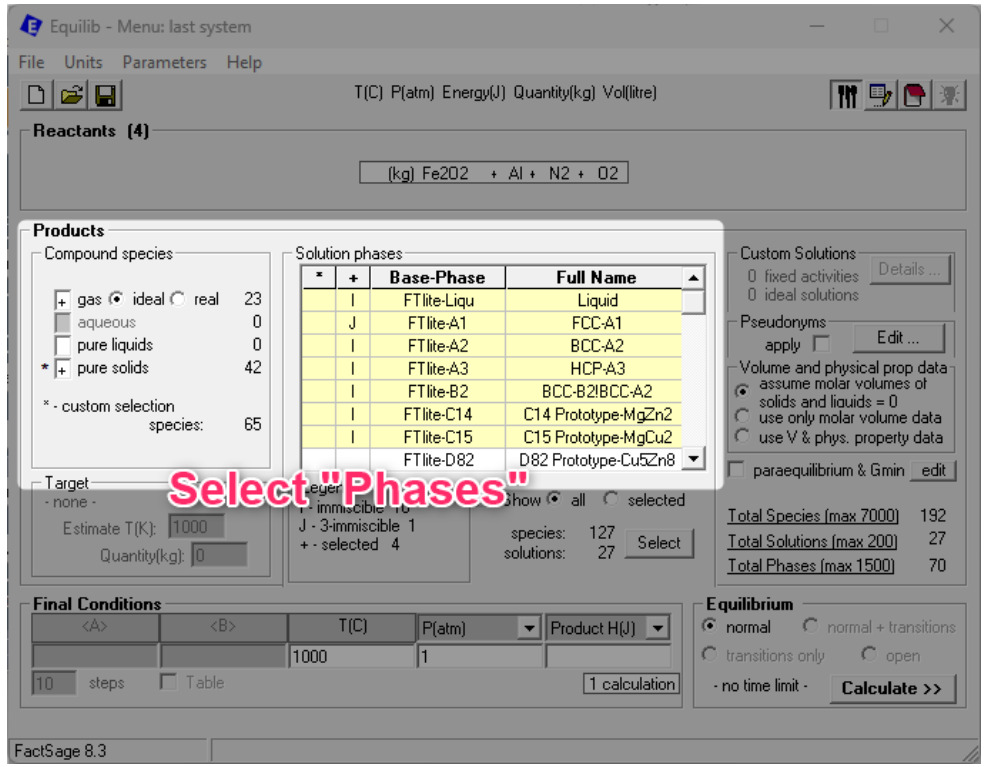
Generate .cst file





3. **Input Species**: Enter the species involved. The quantity values can be arbitrary as they don't impact .cst file generation.

4. **Phase Selection**: Select all phases that may form during the simulation. Note that temperature and pressure settings are not crucial for .cst file generation.

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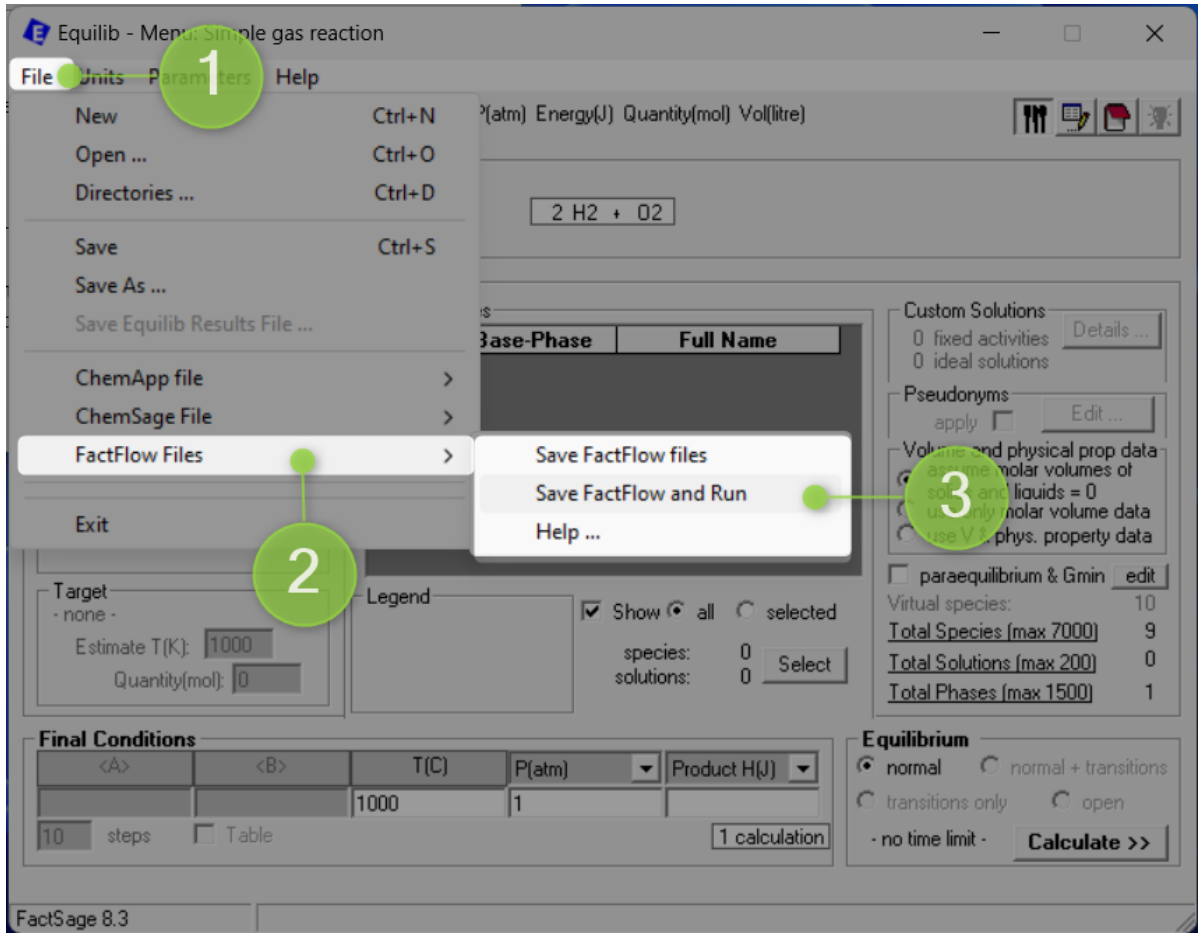
Generate .cst file



5. Saving the File:

Go to [File] > [FactFlow Files] > [Save FactFlow Files] to save the .cst file. Alternatively, choose [Save FactFlow Files and Run] to both save the file and start the FactFlow simulation immediately.

FactFlow

Setup FactFlow

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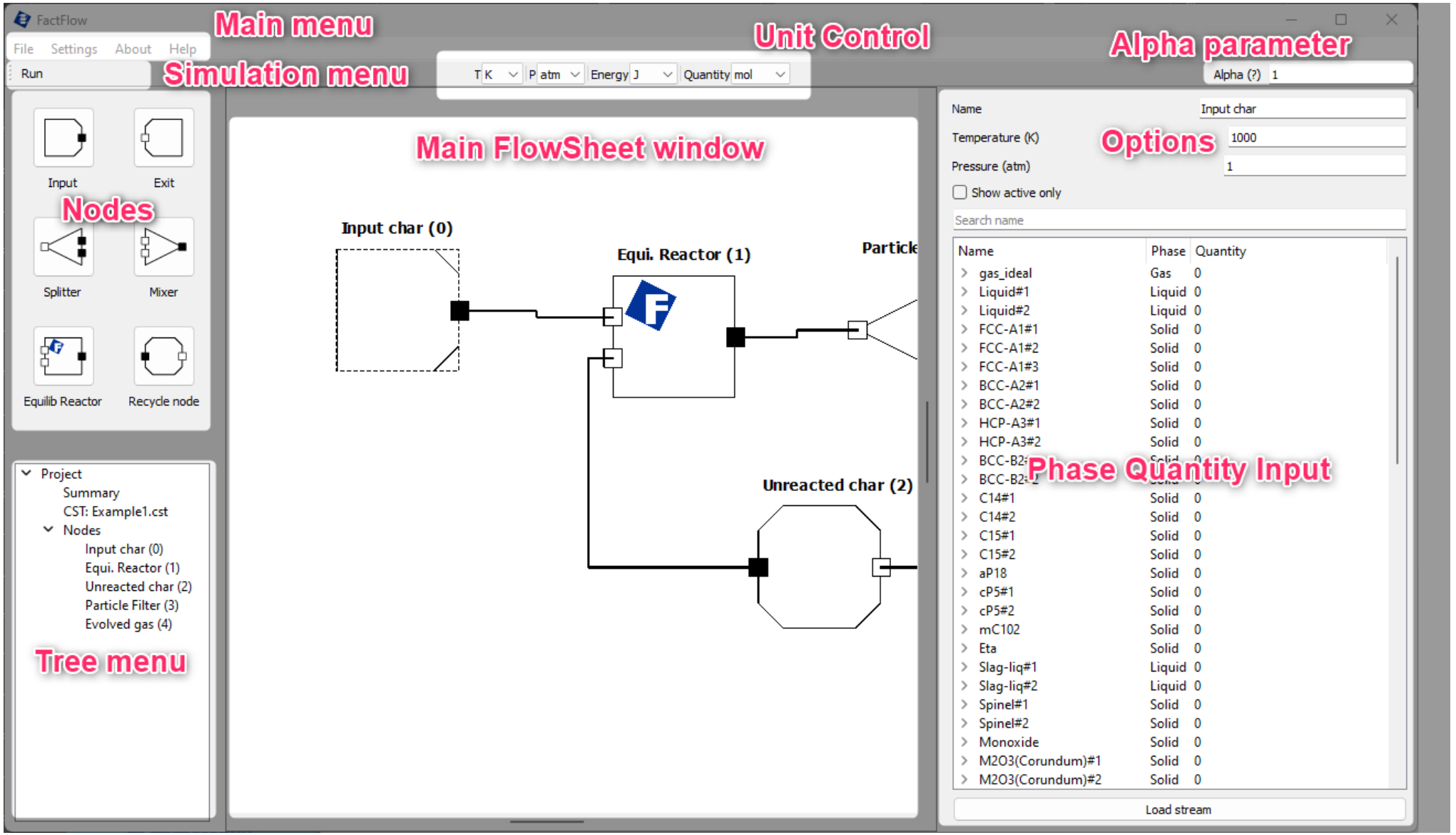
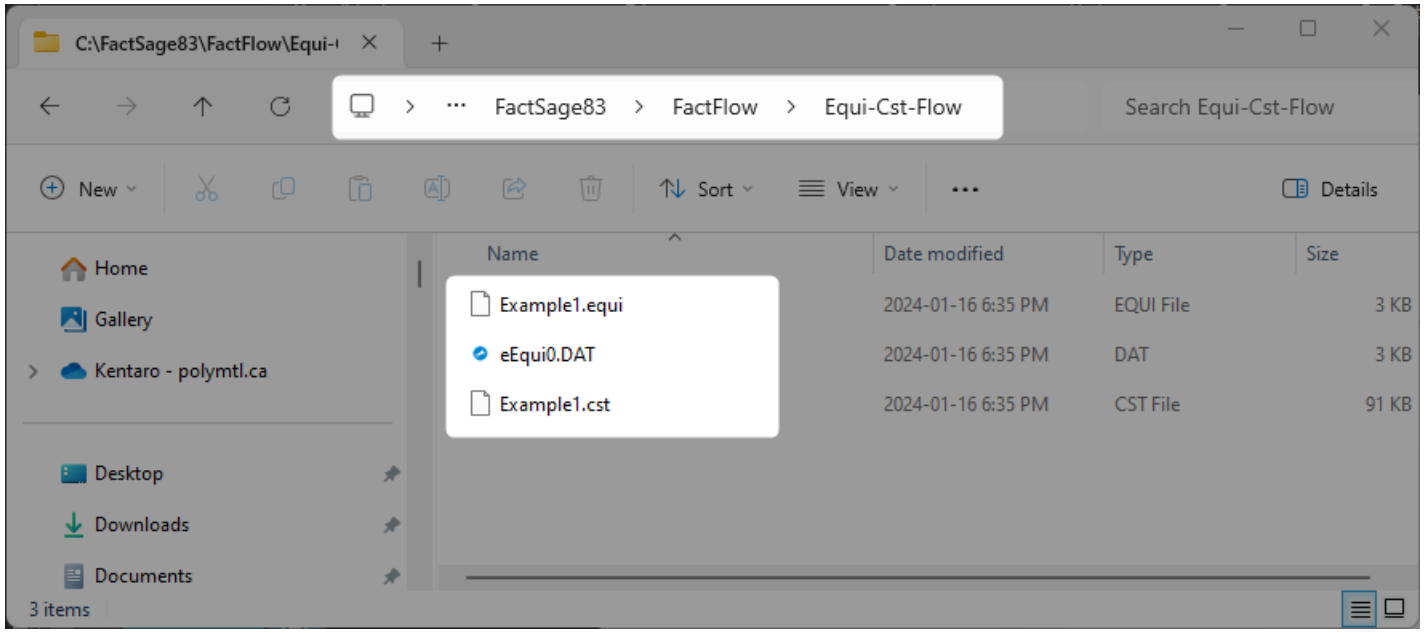
FactFlow Main Interface



Generate .cst file



6. **File Generation Location**: Both .equi and .cst files are created in the [FactSage root]/FactFlow/Equi-Cst-Flow directory.

7. **Editing and Reproducing .cst Files**: Users can modify and regenerate .cst files using the Equilib module. To do this:

    1) Open the Equilib module.
    2) Load the .equi file that needs editing.
    3) Make the necessary changes.
    4) Save the updated settings as a new .cst file.

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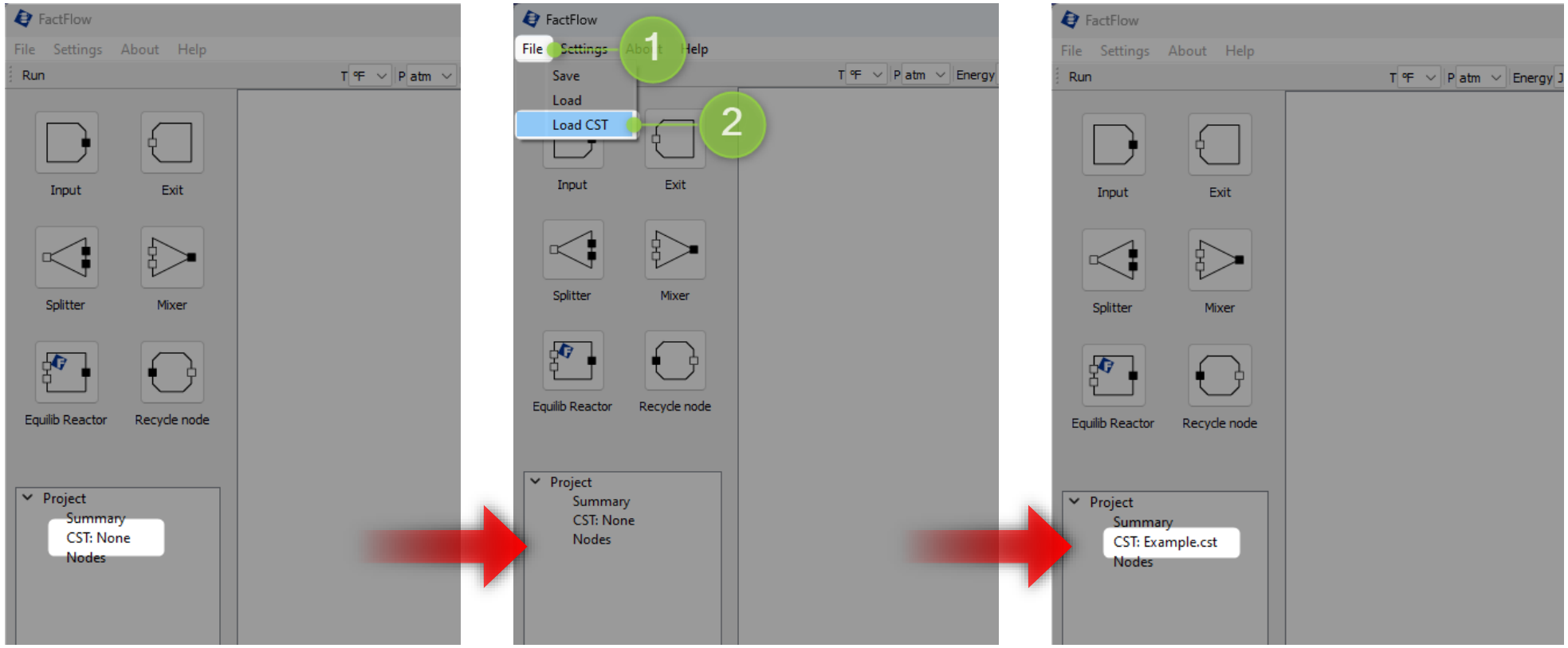
Load .cst file



1. **Check Current File**: Look in the Project Tree menu to see if a .cst file is already loaded.
2. **Load New File**: If no file is loaded, go to [File] > [Load CST], and select your desired .cst file.
3. **Confirm Load**: Once loaded, the .cst file will appear in the Project Tree menu.

FactFlow

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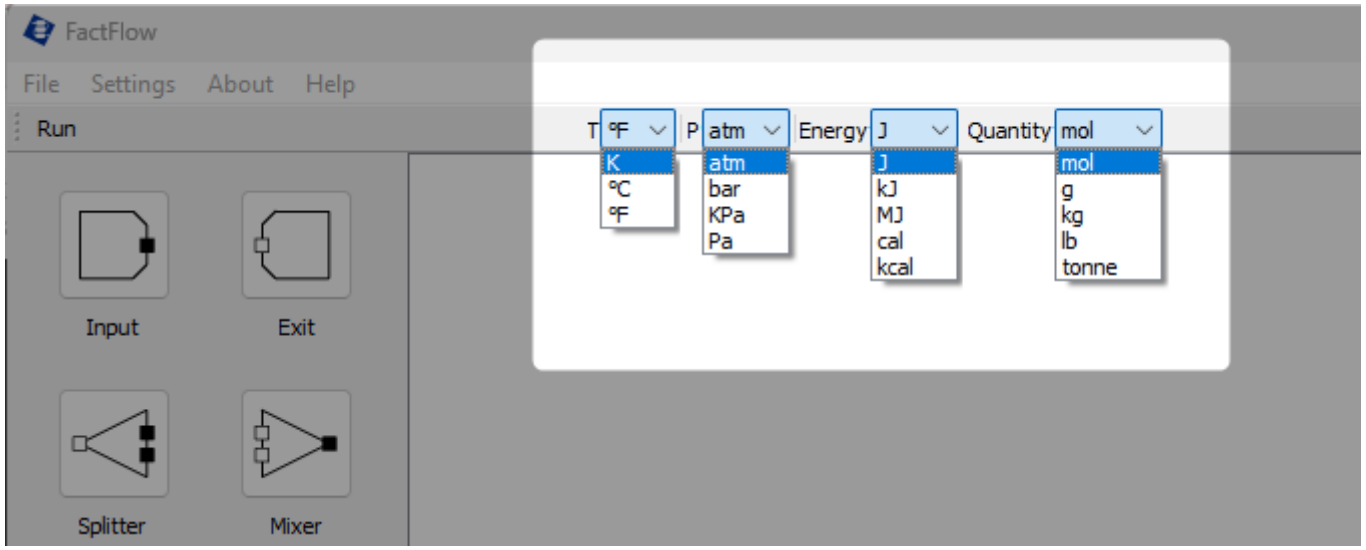
Setup Units



Before starting simulations, it's essential for users to configure their preferred units:

- **Temperature Units**: Kelvin (K), Celsius (^{o}C), or Fahrenheit (^{o}F).
- **Pressure Units**: atmospheres (atm), bars (bar), kilopascals (KPa), or pascals (Pa).
- **Energy Units**: joules (J), kilojoules (kJ), megajoules (MJ), calories (cal), or kilocalories (kcal).
- **Quantity Units**: moles (mol), grams (g), kilograms (kg), pounds (lb), or tonnes (tonne).

FactFlow

Create FactFlow sheet

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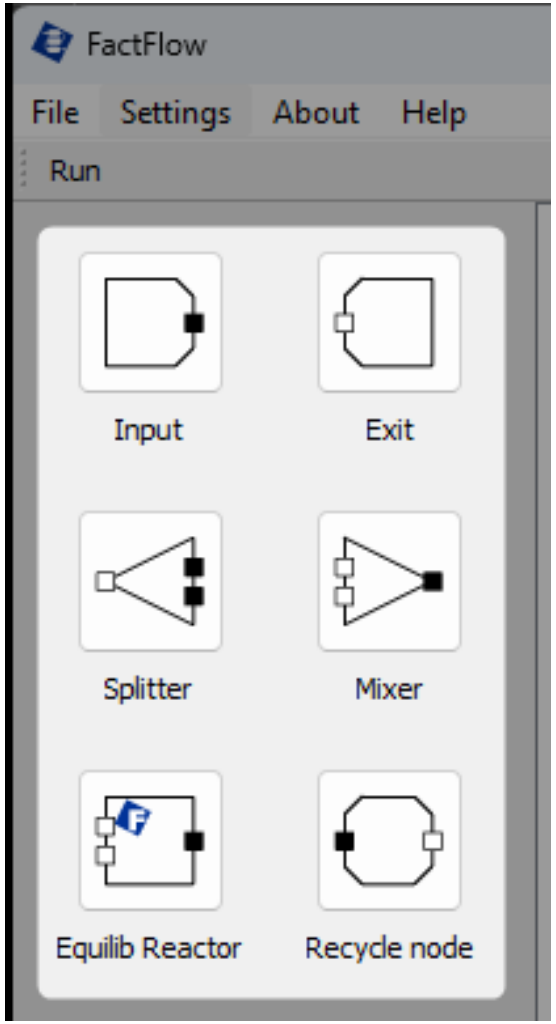
Overview of Node Types



FactFlow includes six distinct node types, each with a specific role:

- **Input**: Sets up and defines the initial input stream, including phase or constituent quantities and initial parameters.
- **Exit**: Retrieves and analyzes output from the simulation, serving as the endpoint for result examination.
- **Splitter**: Divides a stream into parts based on state, flow rate, phases, or gas constituents.
- **Equilib. Reactor**: Conducts equilibrium calculations for chemical processes within the simulation.
- **Recycle**: Reiterates the simulation flow multiple times, useful for processes requiring cycling.

Each node type contributes uniquely to the simulation process, allowing for detailed and customized simulation setups.

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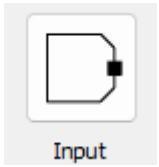
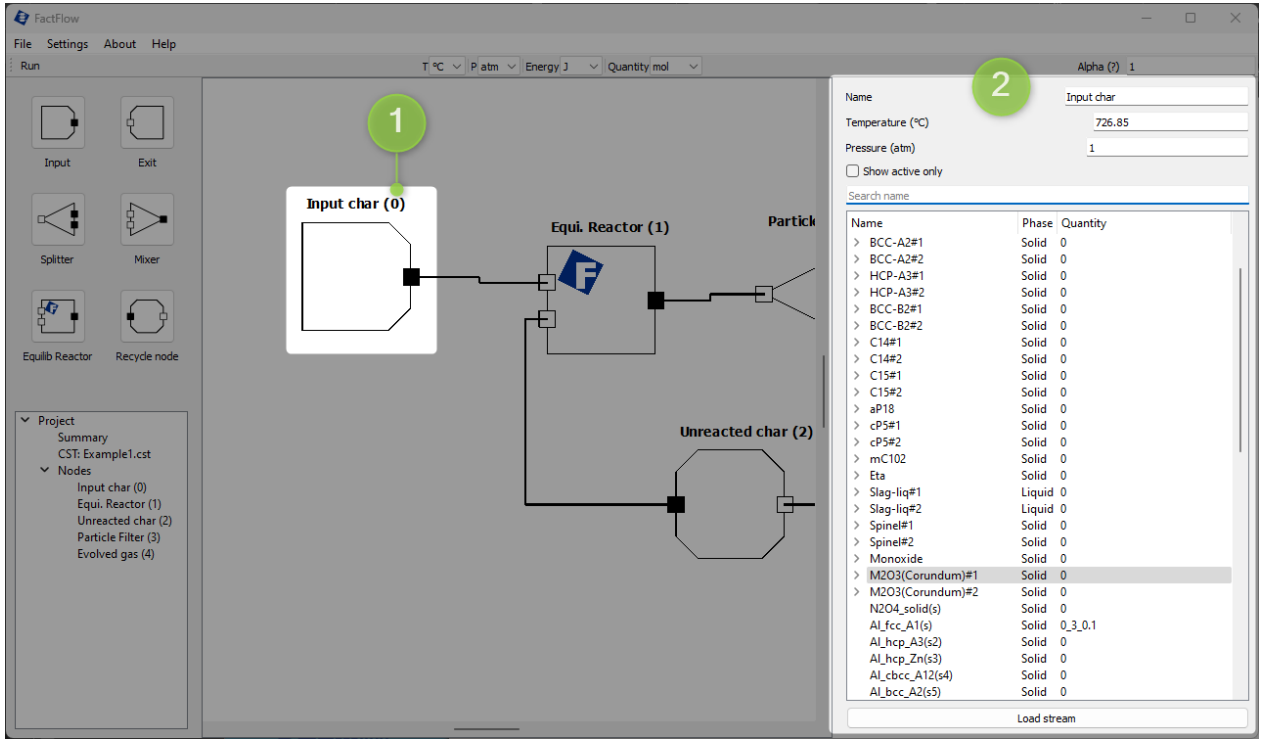


Input node



The Input Node is essential for defining the initial conditions of the simulation:

1. **Editing Access**: Click the node to open the parameter window for modifications.
2. **Setup Parameters**: Configure Node Name, Temperature, Pressure.
3. **Stream Composition**: Set phase or constituent quantities in the input stream.

This node forms the basis for starting the simulation with precise user-defined settings.

FactFlow

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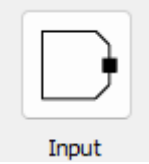
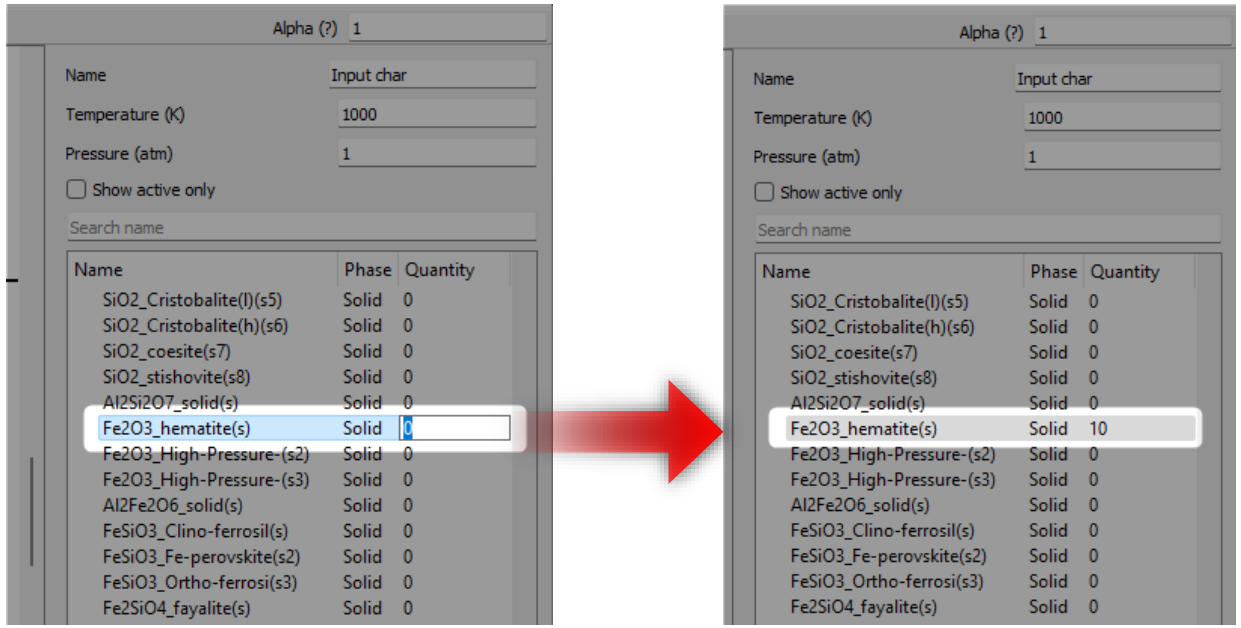


Input node – Enter value



For setting quantities in the Input Node:

1. **Select Phase**: Choose the phase you want to define from the list.
2. **Enter Quantity**: Input the numerical value for the phase in the Quantity column. You can enter values in standard or scientific notation (e.g., 1.2e-6 for 1.2 x 10^(-6)) and press Enter on the keyboard.

This approach allows for precise and flexible input of phase quantities, accommodating various numerical formats.

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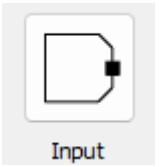
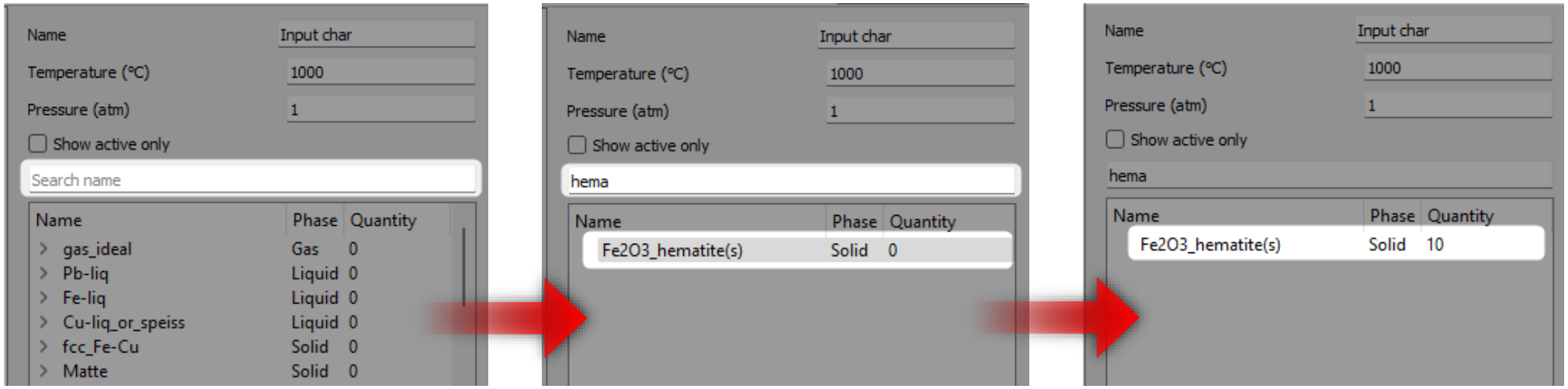


Input node – Search and Enter



To efficiently manage phase or constituent selection and input in the Input Node:

- **Utilize the Search Box**: Found within the Input Node option menu.
- **Search/Filter by Name**: Type the desired phase or constituent's name to quickly locate it. The search is not case sensitive.
- **Input Values**: Once the target phase or constituent is identified, enter its numerical value directly in the Quantity column.

This functionality aids in swiftly identifying and setting the quantities for specific phases or constituents in the simulation's input stream.

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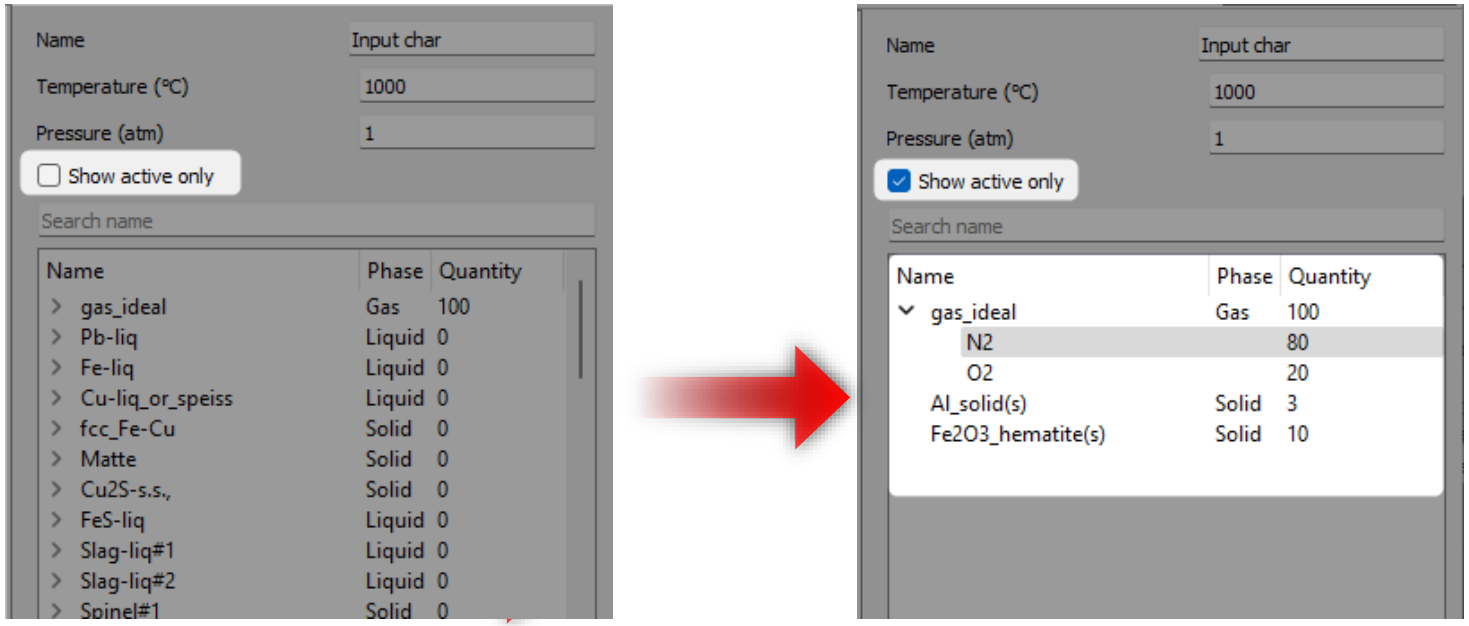
Input node – Active Phases Filter



For users to view only active and valued phases or constituents in the Input Node:

- **Select 'Show Active Only'**: Check the "Show active only" checkbox.
- **Filtered Display**: This shows only phases or constituents with entered values.
- **Assists in Verification**: Useful for ensuring all necessary inputs are properly set.

This function simplifies checking the setup by highlighting active elements in the simulation.

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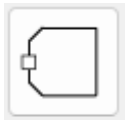
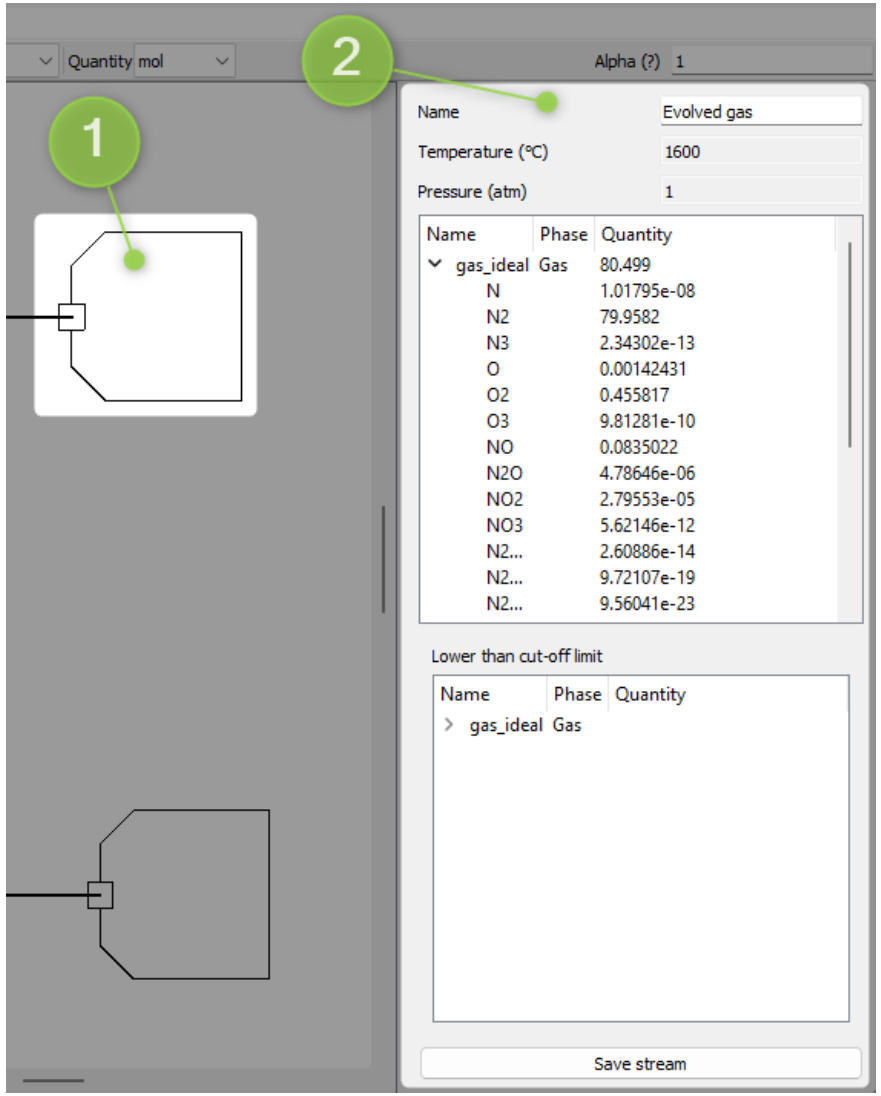


Exit node



The Exit Node is integral in FactFlow for concluding simulations:

- **Role**: It signifies the end of the process flow, allowing for the inspection of the final output stream.
- **Functionality**: This node provides a detailed visualization of the output, listing all constituents and phases at the process's conclusion.
- **Alpha Parameter Results**: It is particularly useful for visualizing outcomes when simulations involve variations using the Alpha parameter.
  See "How to set Alpha parameter" for more details

The Exit Node is essential for analyzing and understanding the final results of the simulated process in FactFlow.

FactFlow

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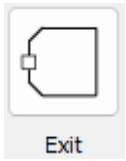
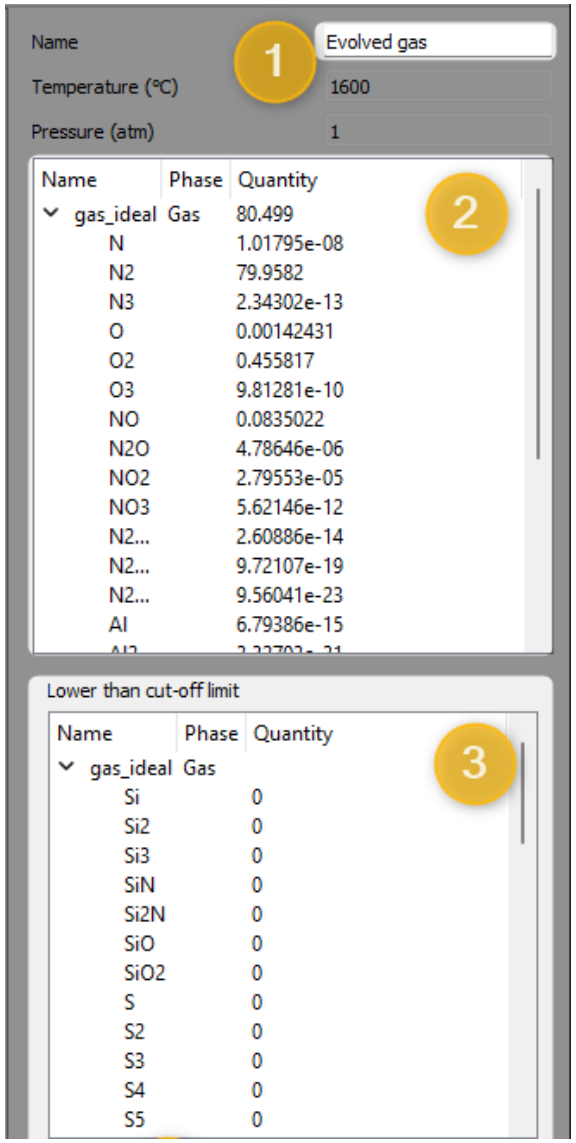
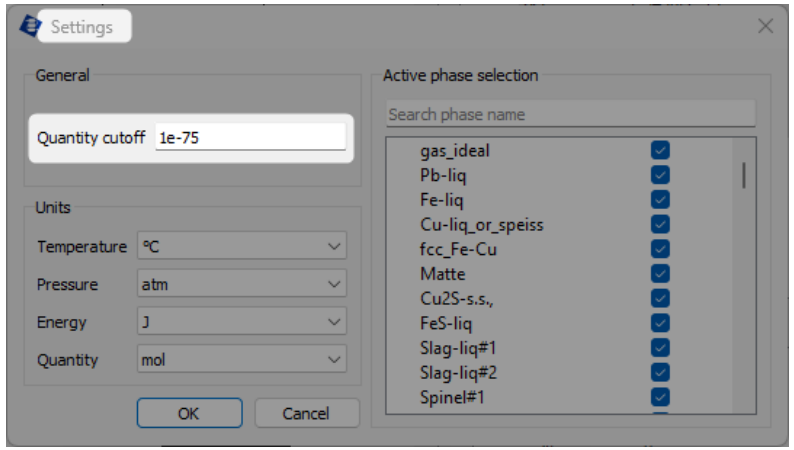


Exit node





- **Edit Node Name**: Allows for the renaming of nodes for clarity.
- **Significant Outputs**: Lists important output phases and constituents above the cut-off threshold.
- **Minor Outputs**: Displays outputs below the cut-off, showing less relevant data.

The cut-off limit, adjustable in Settings, helps streamline output analysis by filtering out less significant data.

FactFlow

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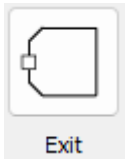
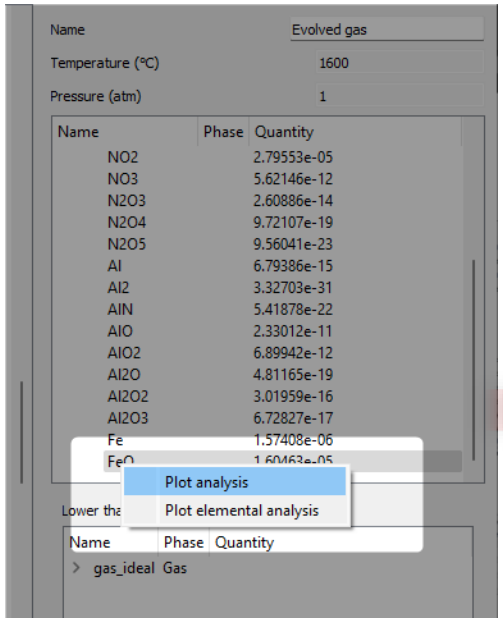
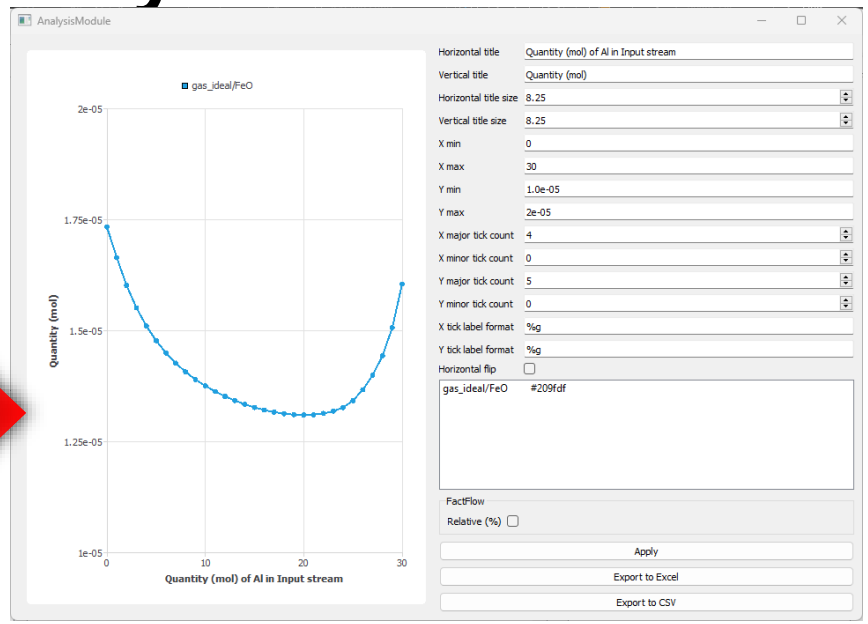


Exit node - Analysis





To begin analyzing simulation outputs from the Exit Node:

- **Access Analysis Functions**: Right-click on the desired phase or constituent from the list within the Exit Node.
- **Select Analysis Option**: Multiple options will be available upon right-clicking.
- **Multiple Selections**: For analyzing several phases or constituents simultaneously, hold down the Ctrl key and click on the desired items.

Please refer to the subsequent slide titled "Analysis Types" for detailed descriptions of the available analysis options.

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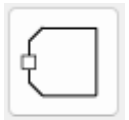
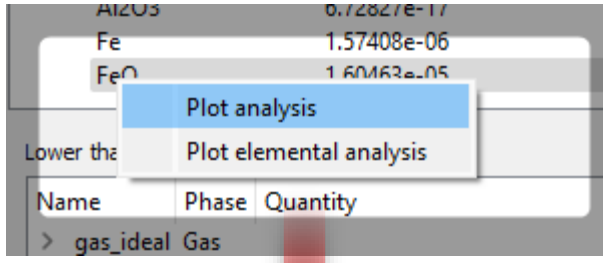
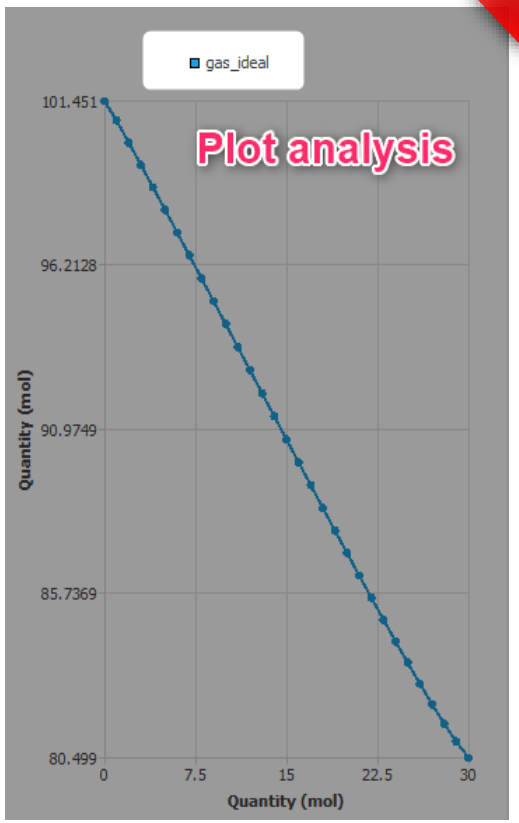
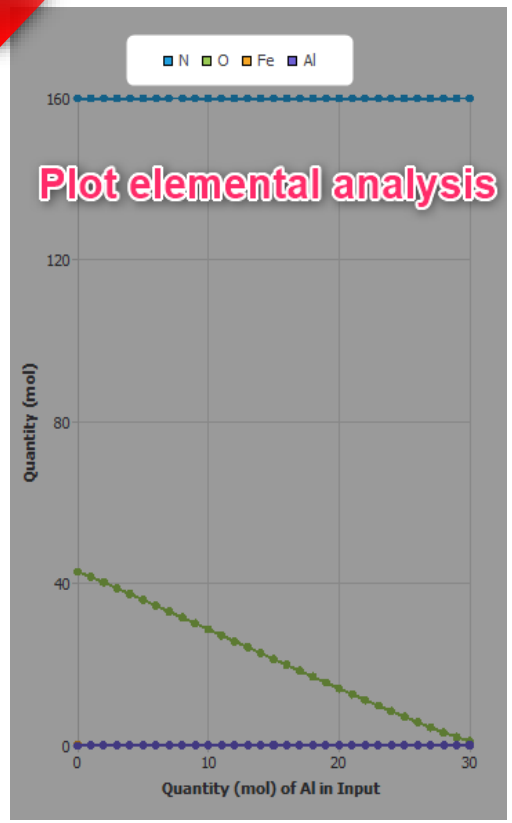


Exit node – Analysis Type







In FactFlow, the Exit Node offers two distinct options for analyzing simulation results:

1. **Plot Analysis**:
   - Graphs phase or constituent quantities versus the alpha parameter.
   - Useful for observing how quantities change with alpha variations.
2. **Plot Elemental Analysis**:
   - Displays a graph of elemental composition within selected phases or constituents.
   - Helps analyze the elemental distribution as affected by the simulation.

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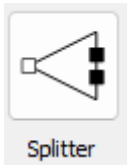
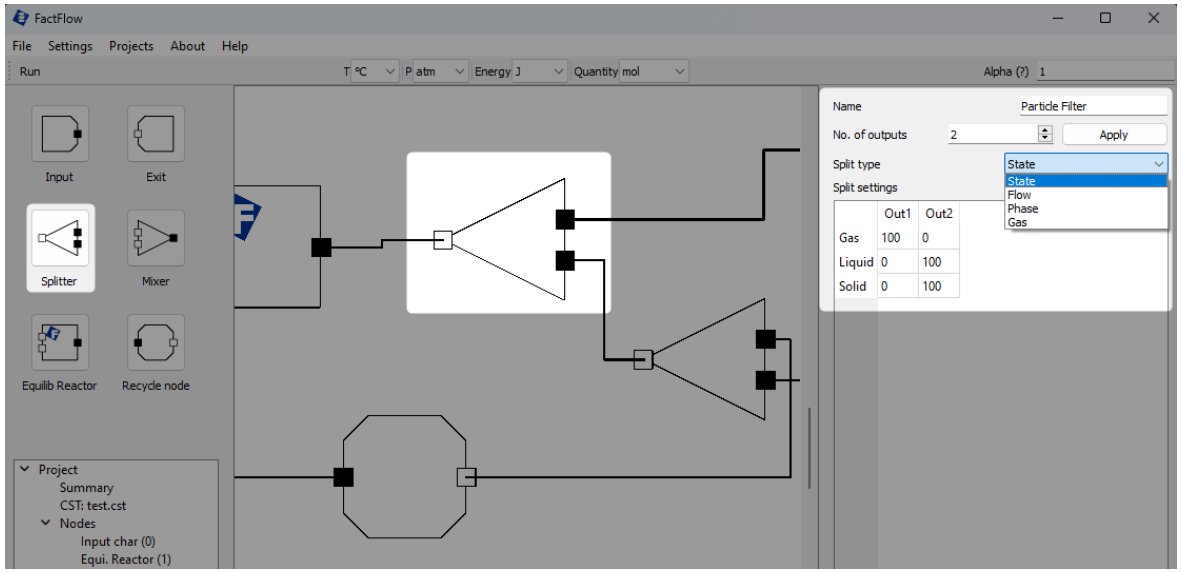


Splitter node



The Splitter Node is designed to bifurcate a process stream within FactFlow:

- **Functionality**: It allows splitting of a stream based on specific criteria such as State, Flow, Phase, or Gas constituent. Further details are provided in the following slide.
- **Node Customization**: Users can edit the name of the Splitter Node for better identification within the simulation workflow.
- **Output Configuration**: The number of desired output streams from the split can be adjusted. Users must input the new number of outputs and click 'Apply' to effect this change.

The Splitter Node's flexibility is crucial for customizing the flow of the simulation to suit complex process requirements.

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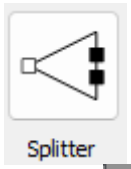
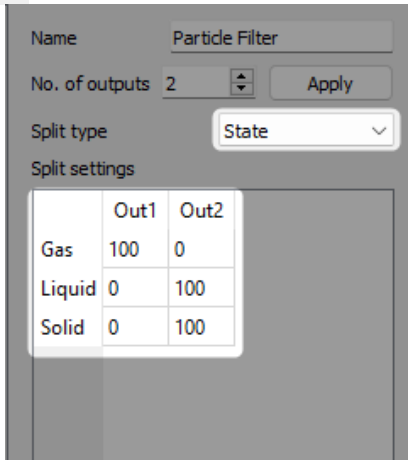
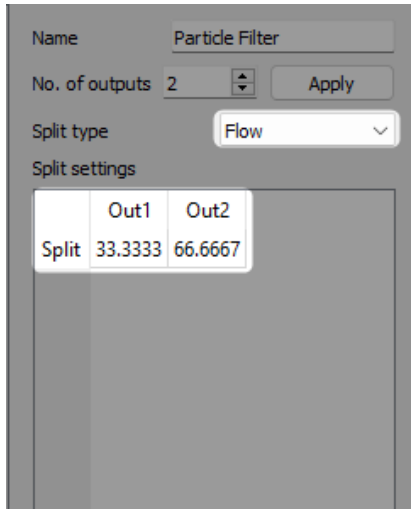
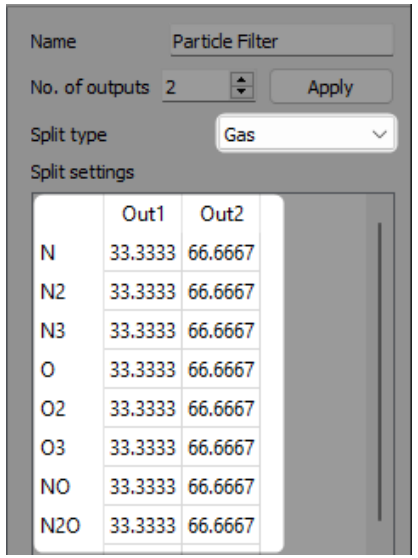
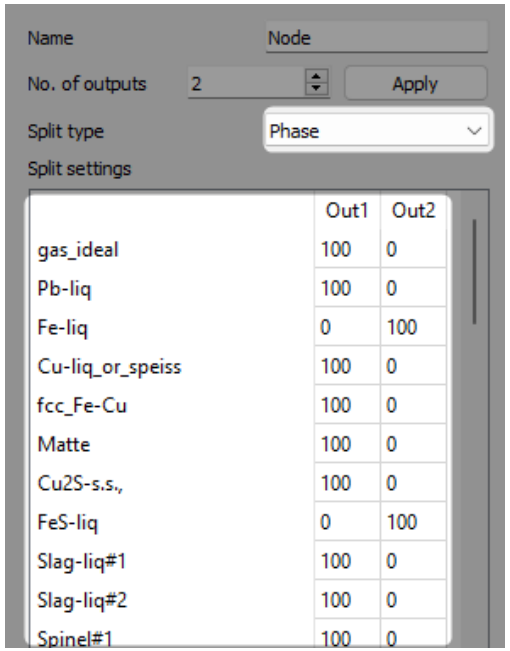


Splitter node – Splitter Type









The Splitter Node offers several options for segmenting process streams:

- **State**: Separates streams by state (gas, liquid, solid).
- **Flow**: Divides streams by flow quantity, keeping concentration constant.
- **Gas**: Segregates specific gas constituents, affecting equilibrium state.
- **Phase**: Splits streams by distinct phases for separate processing.

Note: Gas splitting alters the stream from its equilibrium state, which is crucial for subsequent simulation analysis.

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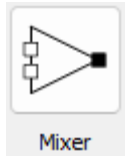
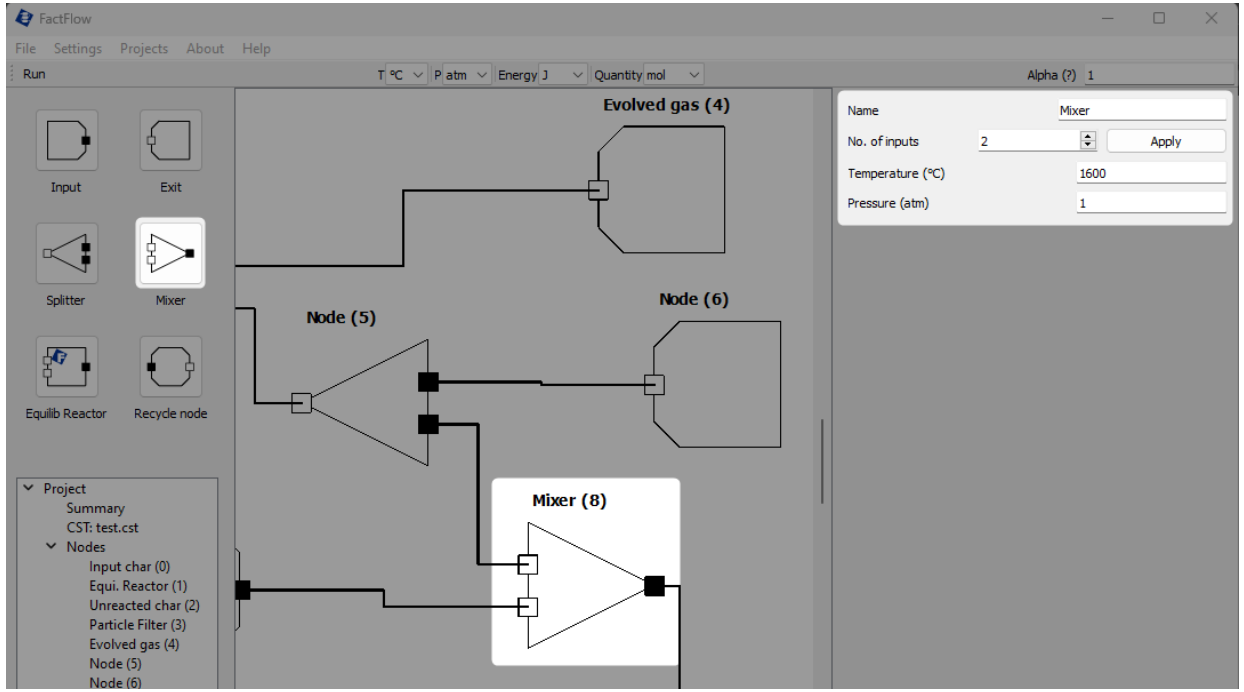


Mixer node



The Mixer Node in FactFlow is designed for combining multiple streams:

- **Temperature and Pressure Input**: Users set the mixer's temperature; however, equilibrium calculations are not performed.
- **Node Name Customization**: Allows users to rename the node for clarity.
- **Input Stream Adjustment**: Users can set and modify the number of input streams; changes are applied by clicking 'Apply'.

Note: The output stream from the Mixer Node may not be in equilibrium.

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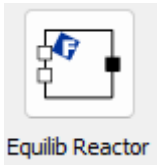
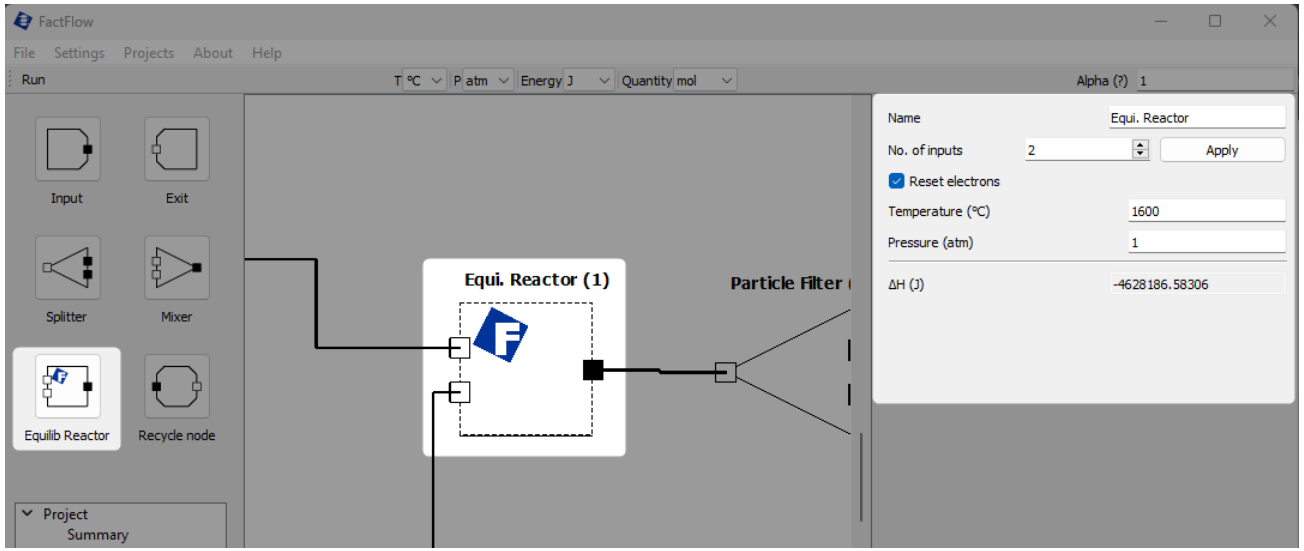


Equilib node



The Equilib Node is a critical component in FactFlow for equilibrium calculations:

- **Equilibrium Calculations**: Executes Gibbs energy minimization, similar to FactSage's Equilib module.
- **Node Name Customization**: Allows users to rename the node for better identification in the workflow.
- **Temperature and Pressure Settings**: Users must accurately define temperature and pressure for the calculations.
- **Input Stream Adjustment**: Offers the ability to modify the number of input streams to the node.

The Equilib Node is key for conducting precise thermodynamic equilibrium analyses in simulations.

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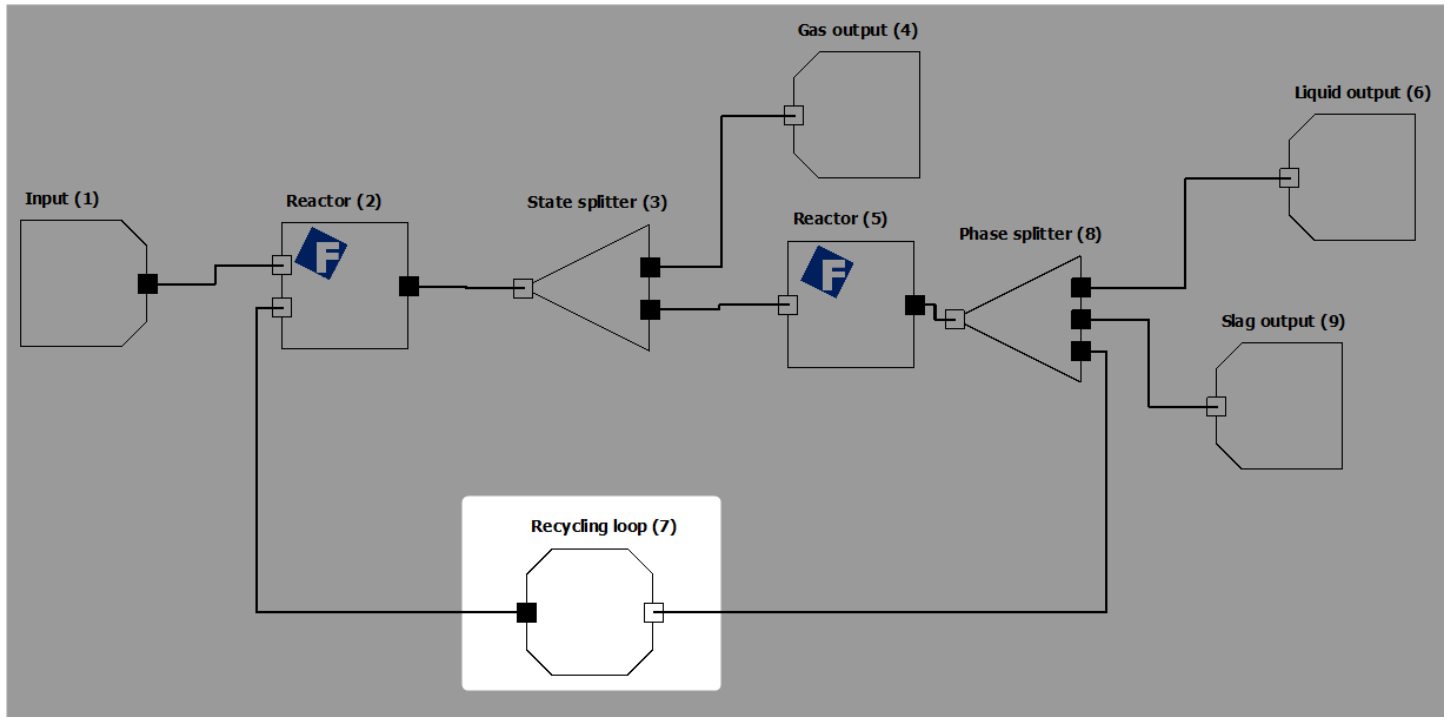
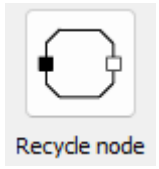
Recycle node

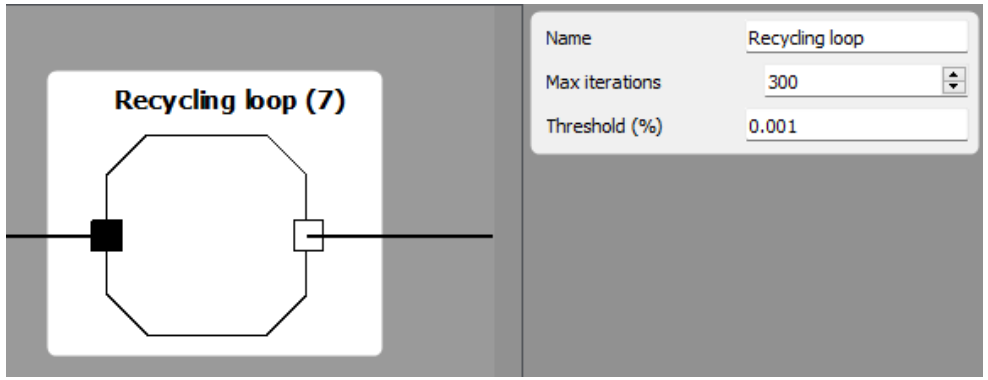


The Recycle Node in FactFlow allows users to redirect part of an output stream back as an input to a previously calculated node, facilitating iterative recalculations to reach convergence.

The Recycle Node is essential for simulations requiring iterative feedback loops, ensuring that all phases and constituents stabilize according to user-defined criteria.



Recycle node



Maximum Iterations: Users can specify the maximum number of iterations for the recycling process to ensure the simulation remains computationally manageable.

Threshold Setting: The threshold determines when the recycling loop can stop based on the change in the quantity of each phase or constituent between iterations. The recycling process persists as long as the percentage difference in quantities between consecutive iterations surpasses the set threshold. The loop concludes once the percentage variation for every composition falls beneath this threshold, or the preset maximum iteration count is attained.

$$\text{Threshold (\%)} > \frac{m_{i,n}}{m_{i,n-1}} \times 100$$

Here, $m_{i,n}$ represents the quantity of phase or constituent i at iteration n, and $m_{i,n-1}$ is the quantity at the previous iteration, $n-1$. The loop continues until this percentage difference for all phases and constituents falls below the user-set threshold, or until reaching the maximum number of iterations specified.

FactFlow

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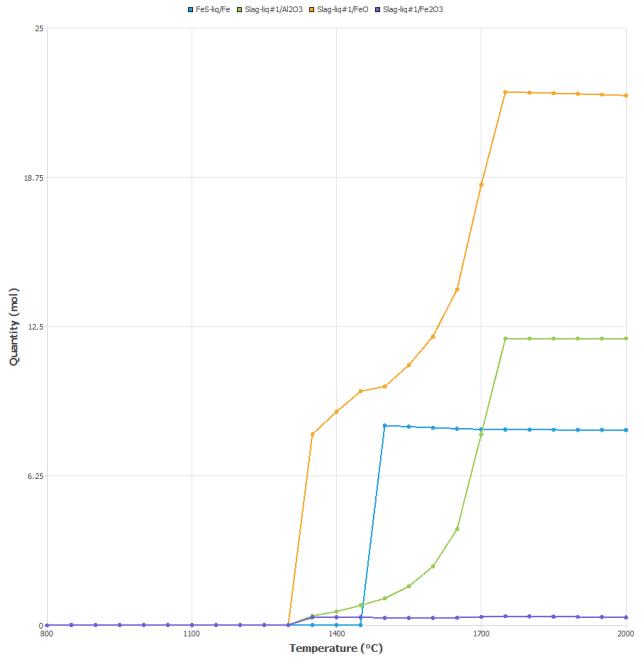
Variable – Alpha parameter



The Alpha parameter in FactFlow is a unique tool designed for varying simulation conditions:

- **Purpose of Alpha Parameter**: It allows users to systematically change and analyze the effects of varying a specific input (such as temperature, pressure, or phase/constituent quantity) within the simulation.
- **Limitation**: Only one Alpha parameter can be set for the entire simulation. This ensures focused and clear results from varying a single input across a defined range.

The Alpha parameter is integral for simulations requiring detailed analysis of how changes in one variable can influence the overall system behavior.

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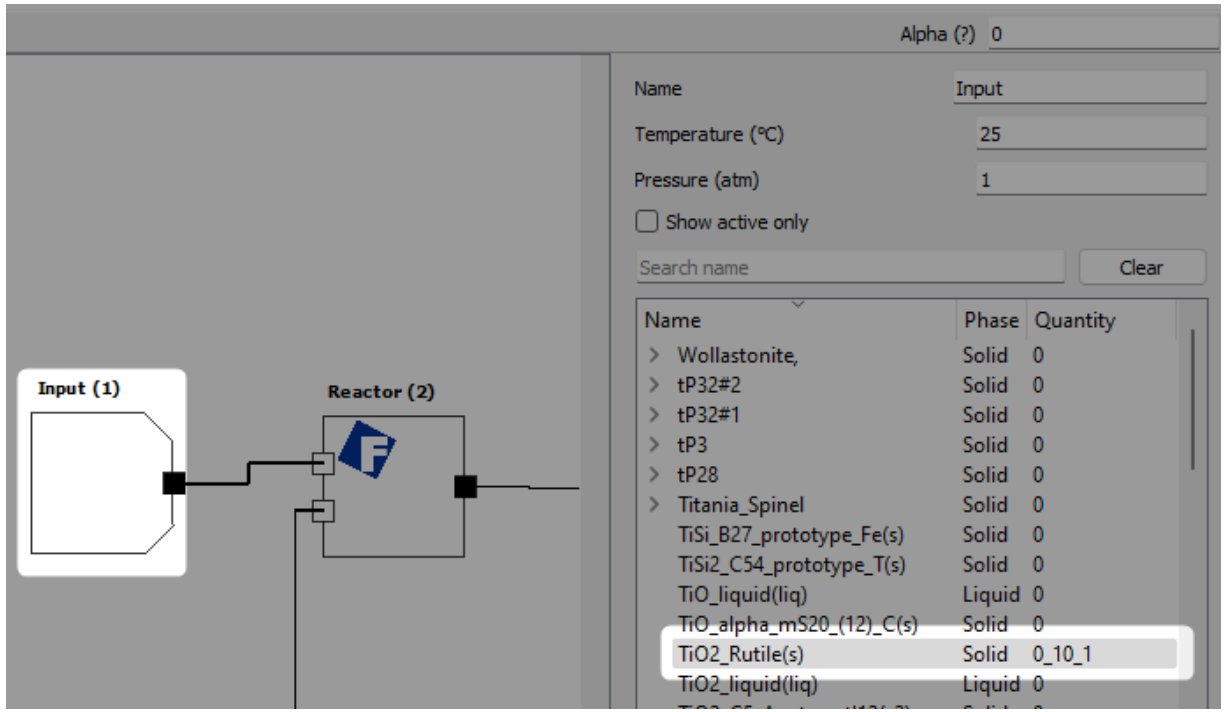
How to set Alpha parameter



FactFlow allows the alpha parameter to be set in two distinct ways, enabling users to systematically vary inputs across simulations:

1. Direct Input Method: Users directly enter the alpha parameter values in the format of **minimum_maximum_step** in the input field. For instance, specifying "0_10_1" indicates that the quantity of a phase or constituent (e.g., TiO2_Rutile(s)) will vary from 0 to 10 with increments of 1 mole, resulting in 11 calculation variations. This method applies to phase or constituent quantities, as well as Temperature and Pressure settings.

FactFlow

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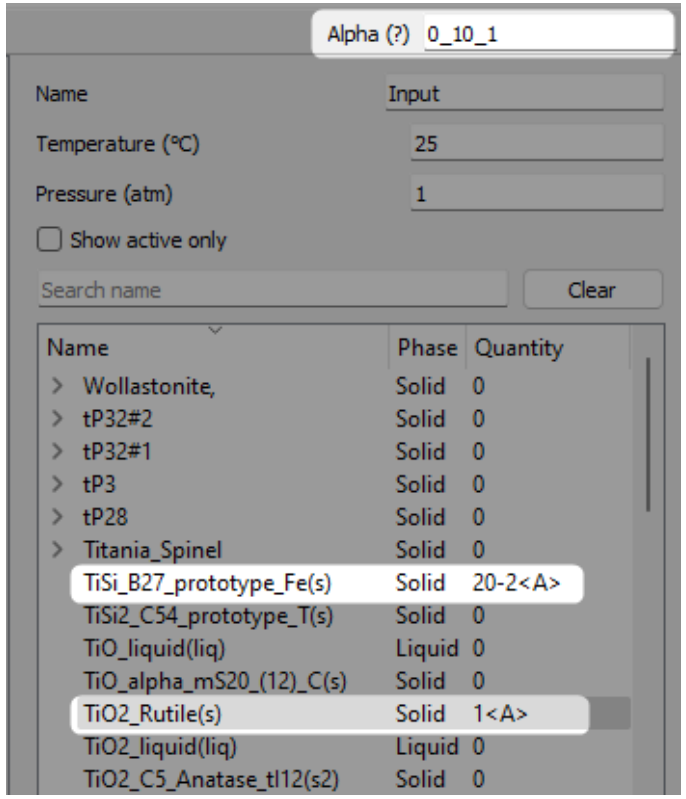
How to set Alpha parameter



2. Placeholder Method: By entering "<A>" in the input field, users can then specify the alpha parameter values in a separate input field labeled 'Alpha', located at the top right corner of the FactFlow interface. This approach allows for the alpha parameter to be applied across multiple phases or constituents. For example, using the notation "20-2<A>" with the alpha parameter set to "0_10_1" means the quantity of TiSi-B27 will decrease from 20 moles in steps of 2 moles down to 0, encompassing variations in quantities driven by the alpha parameter.

These methods provide flexibility in conducting parametric studies within simulations, allowing for a detailed exploration of how variations in quantities, temperature, or pressure affect the process's behavior.

FactFlow

Run Simulation

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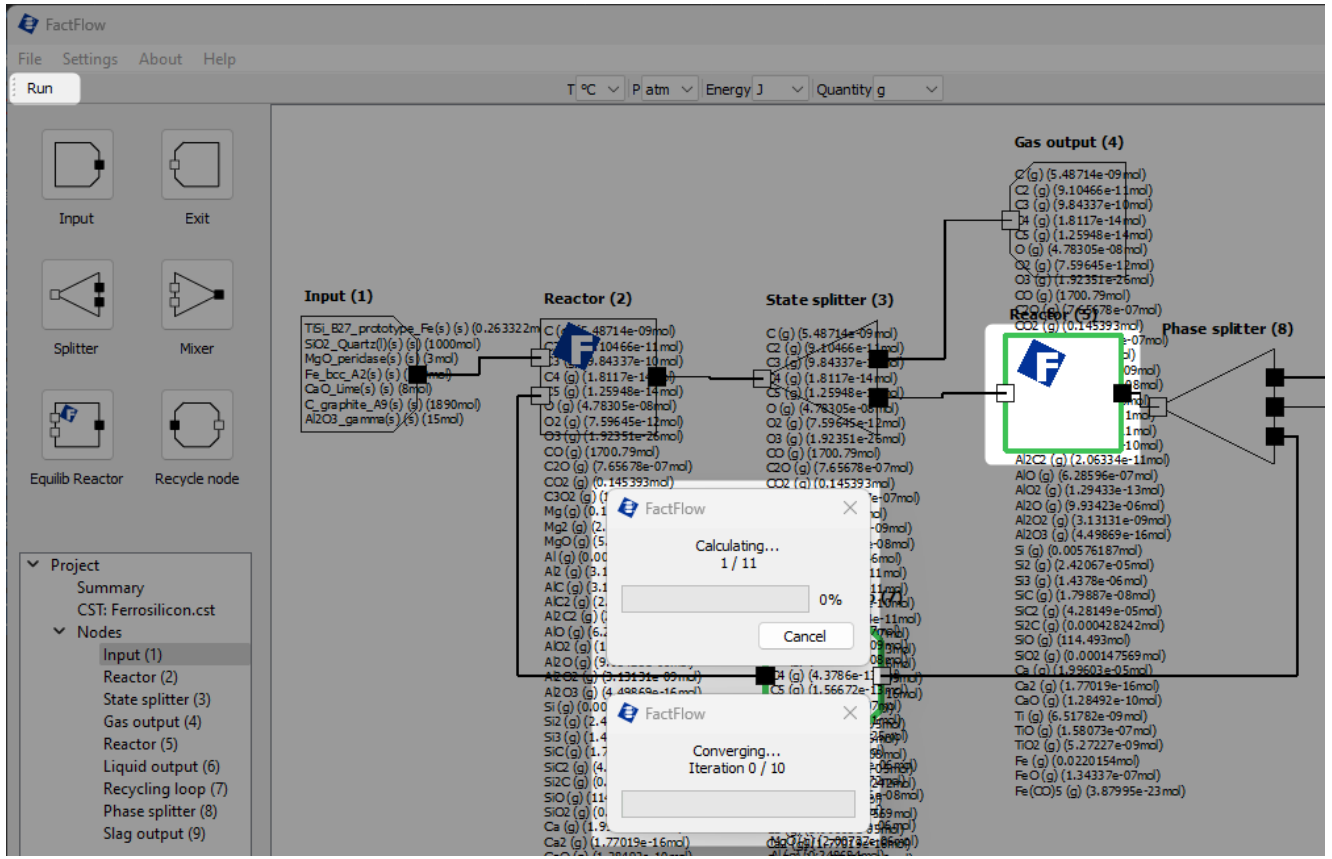
Run simulation



To initiate a simulation in FactFlow after completing the process flow sheet setup:

1. Start the Simulation: Click the "Run" button. This action triggers the simulation to start, processing the defined flow sheet.

Run simulation

2.Visualization of Calculation Process: Nodes currently being calculated are highlighted in green. This visual cue helps users track the progress of the simulation in real-time.

3.Loop Node/Alpha Parameter Calculations: If your simulation includes loop nodes or utilizes the Alpha parameter, a pop-up window will appear, displaying the current progress status of these calculations. This feature provides insights into the iterative or parametric steps of the simulation.

4.Terminating the Simulation: Should you need to halt the calculation process for any reason, you can do so by clicking "Cancel" on the pop-up window. This option allows users to stop the simulation if adjustments or reconfigurations are needed.

This streamlined process ensures users can efficiently run simulations and have control over the calculation progress, including the ability to terminate if necessary.

FactFlow

Analysis

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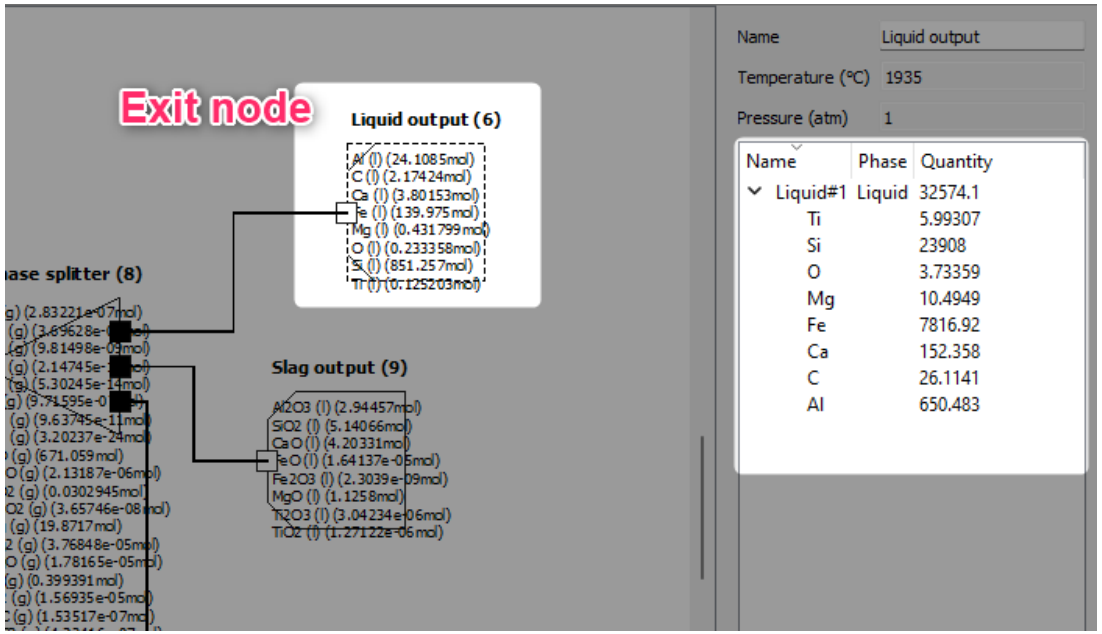
Analyze the results



FactFlow offers two primary methods for users to access and analyze simulation results.

Via the Exit Node:

- Accessing Results: After the simulation completes, click on the Exit Node.
- Result Display: The outcomes will be shown on the right side of the FactFlow interface, providing a straightforward overview of the simulation's end state.

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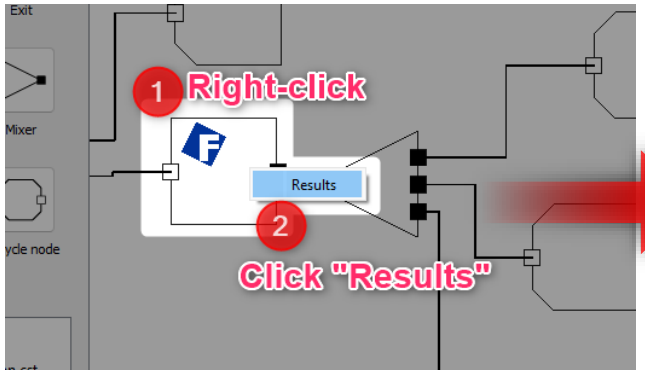
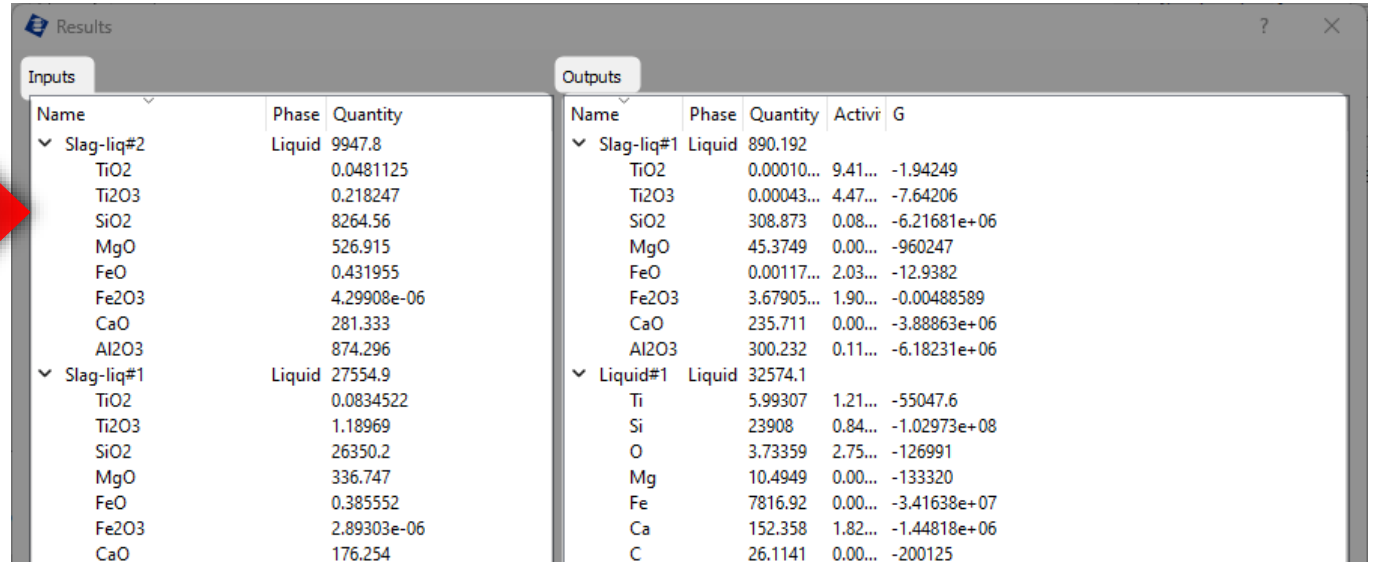
Analyze the results





Name	Phase	Quantity
Slag-liq#2	Liquid	9947.8
TiO2		0.0481125
Ti2O3		0.218247
SiO2		8264.56
MgO		526.915
FeO		0.431955
Fe2O3		4.29908e-06
CaO		281.333
Al2O3		874.296
Slag-liq#1	Liquid	27554.9
TiO2		0.0834522
Ti2O3		1.18969
SiO2		26350.2
MgO		336.747
FeO		0.385552
Fe2O3		2.89303e-06
CaO		176.254

Name	Phase	Quantity	Activi	G
Slag-liq#1	Liquid	890.192		
TiO2		0.00010...	9.41...	-1.94249
Ti2O3		0.00043...	4.47...	-7.64206
SiO2		308.873	0.08...	-6.21681e+06
MgO		45.3749	0.00...	-960247
FeO		0.00117...	2.03...	-12.9382
Fe2O3		3.67905...	1.90...	-0.00488589
CaO		235.711	0.00...	-3.88863e+06
Al2O3		300.232	0.11...	-6.18231e+06
Liquid#1	Liquid	32574.1		
Ti		5.99307	1.21...	-55047.6
Si		23908	0.84...	-1.02973e+08
O		3.73359	2.75...	-126991
Mg		10.4949	0.00...	-133320
Fe		7816.92	0.00...	-3.41638e+07
Ca		152.358	1.82...	-1.44818e+06
C		26.1141	0.00...	-200125

Via the Equilib Node:

- Investigating Results: Right-click on the Equilib Node you wish to examine.
- Accessing Detailed Results: From the context menu that appears, select "Results". A new pop-up window will display both the input parameters and the output of the equilibrium calculations performed by FactSage, offering detailed insights into the equilibrium state achieved in the simulation.

These approaches allow users to effectively analyze the results, whether looking for a quick overview via the Exit Node or delving into detailed equilibrium analysis via the Equilib Node.

FactFlow

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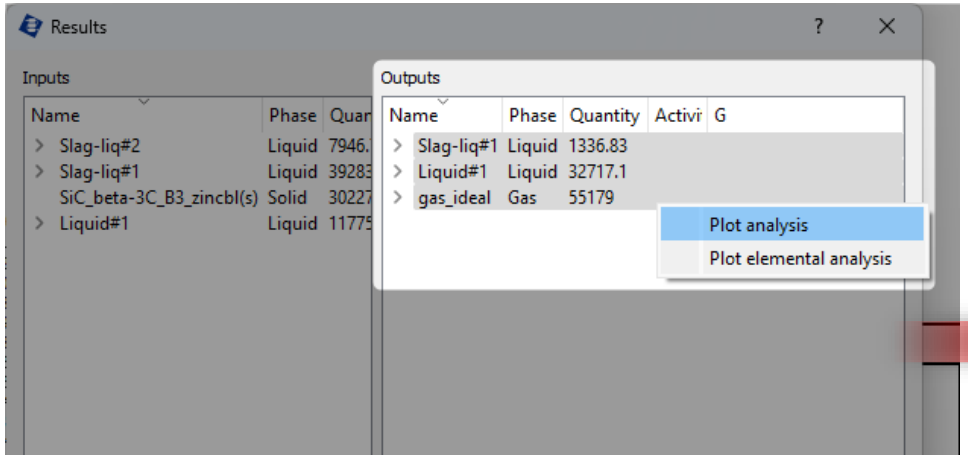
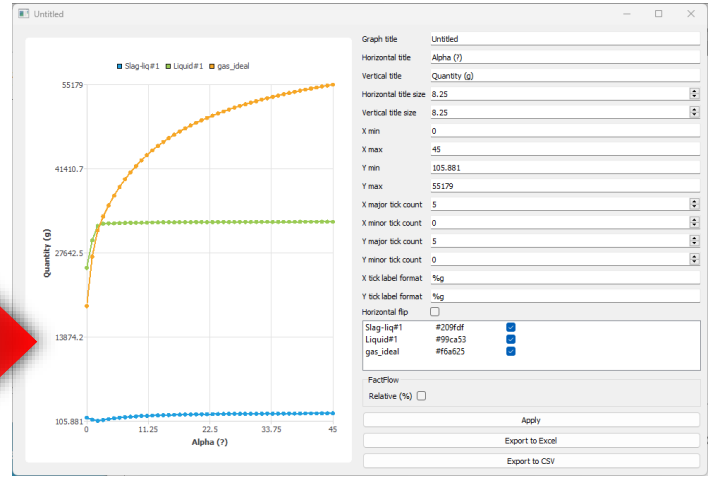
Visualization of results





To visualize simulation results in FactFlow:

- **Navigate to Outputs**: Go to the outputs of either an Equilib Node or Exit Node.
- **Select for Analysis**: Click on a phase or constituent for analysis. For multiple selections, use 'Ctrl + Click'.
- **Analysis Options**:
  - Plot Analysis: Visualizes the selected phases or constituents versus the Alpha parameter.
  - Plot Elemental Analysis: Shows the total elemental amounts in selected phases, revealing variations with the Alpha parameter.

These steps enable clear and concise visualization of simulation data, assisting in the detailed examination of simulation outcomes.

FactFlow

Data Export

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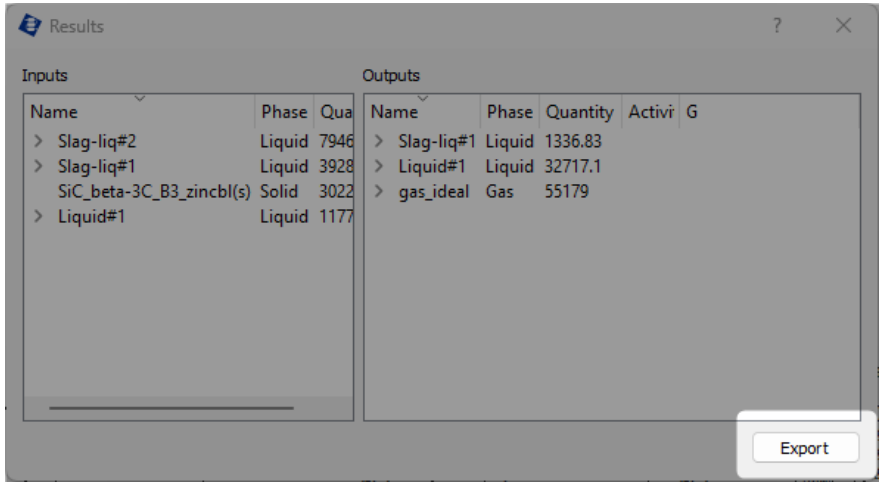
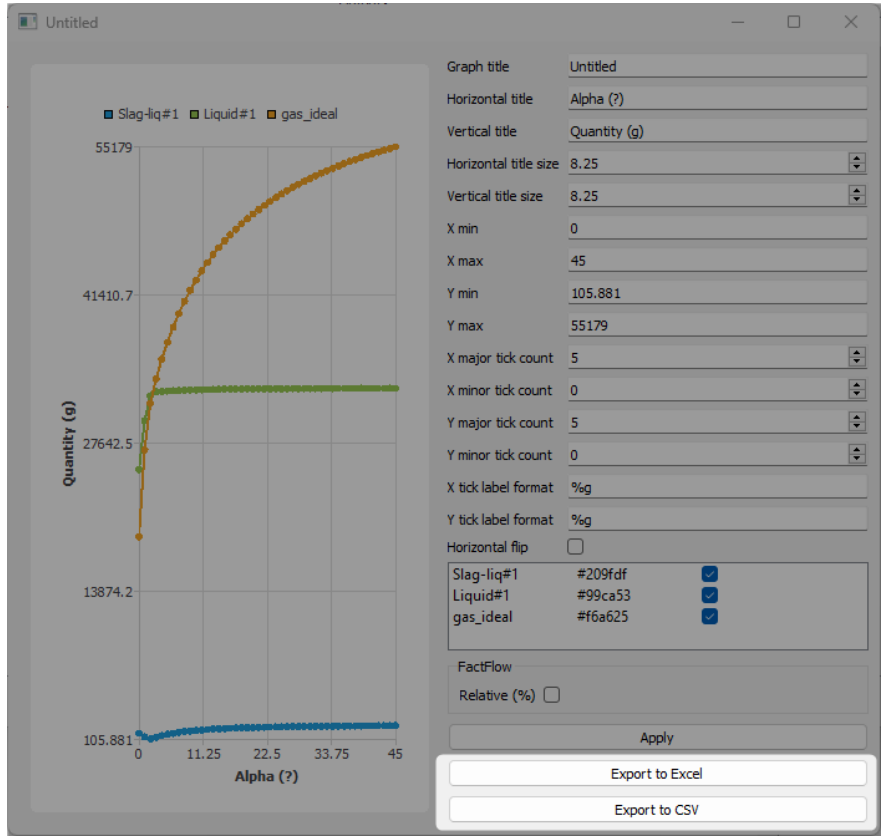
Export the results





Exporting Equilib Calculation Results:

- Navigate to the desired Equilib Node and click the "Export" button. This action enables the export of the equilibrium calculation results directly from the node.

Exporting Plots:

- Users have the option to export plots generated from analyses in either Excel format or CSV format.

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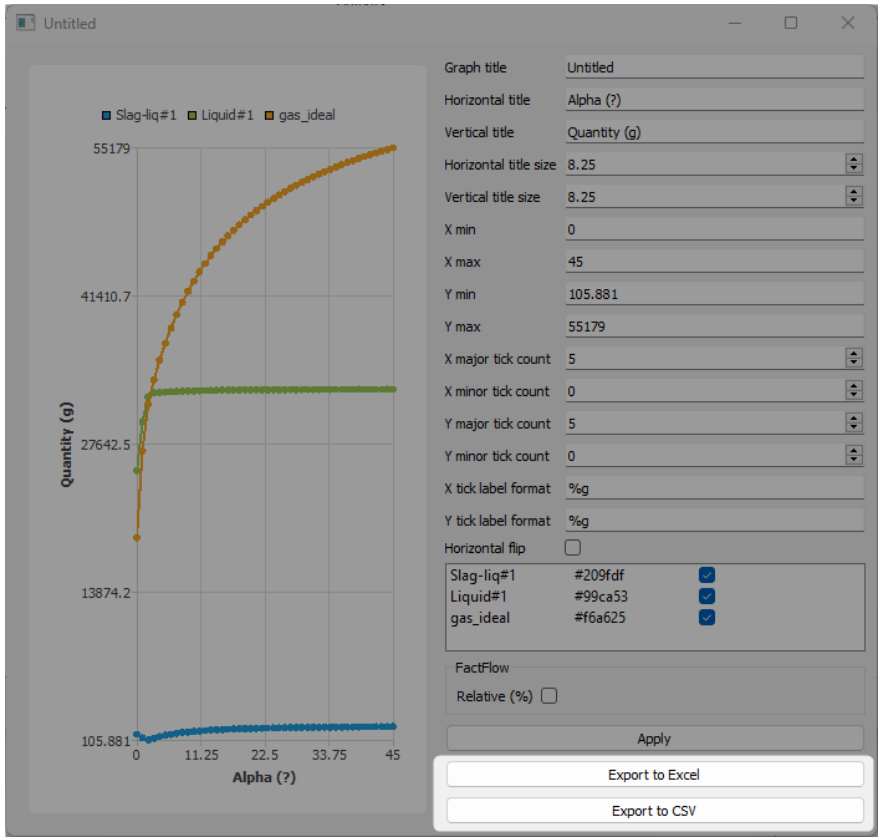
Export the results



Exporting Plots:

- Users have the option to export plots generated from analyses in either Excel format or CSV format.

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Support

Should you encounter any issues, have suggestions, or wish to make recommendations, please do not hesitate to reach out. Send your queries or feedback via email to factflow@polymtl.ca.

Our team is dedicated to providing assistance and improving your experience with FactFlow.