

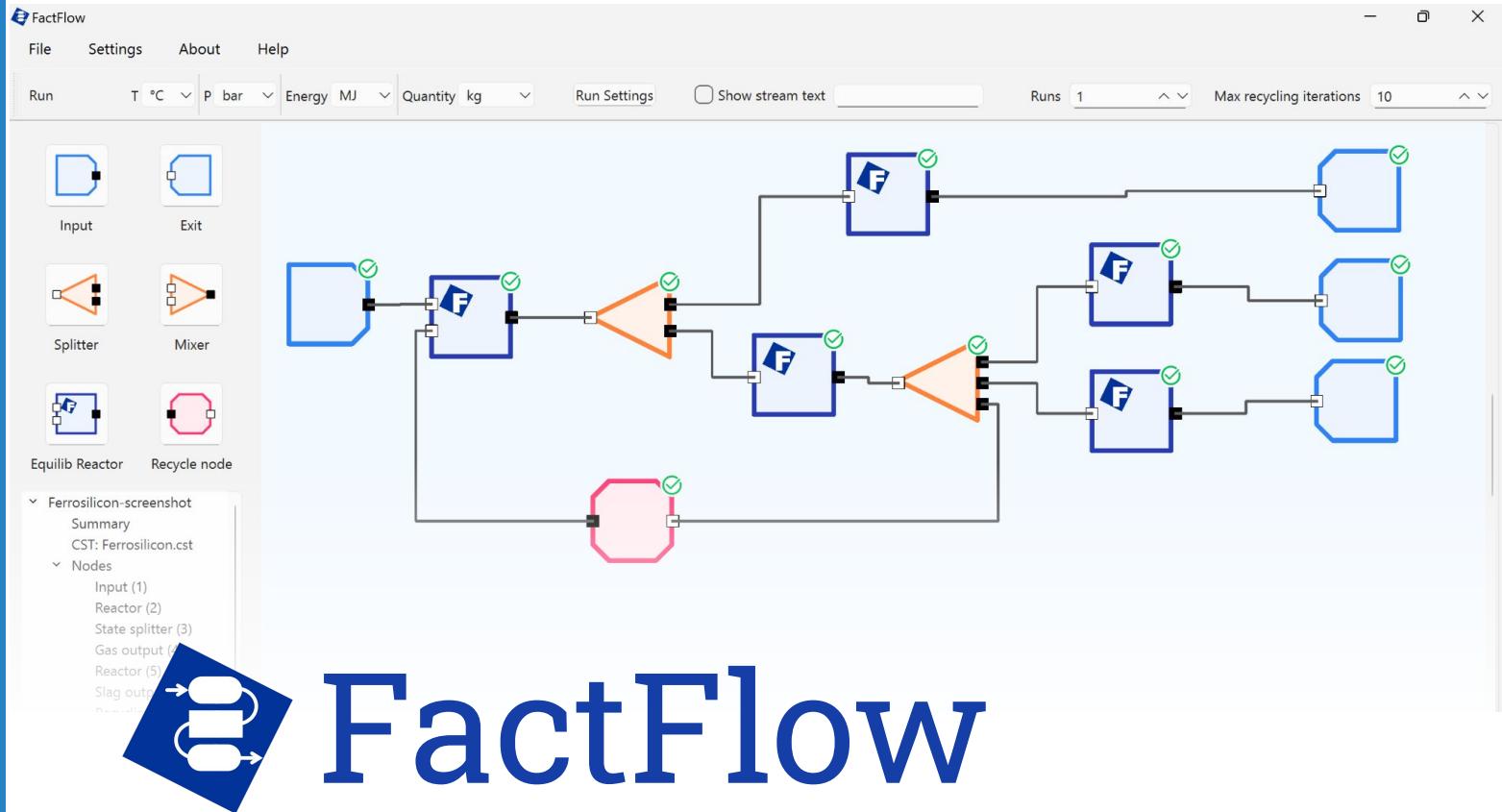


# FactFlow

## User manual

- What is FactFlow?
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# FactFlow User manual



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# What is FactFlow?

**FactFlow** is FactSage's new process simulation and optimization interface.

## Key features include:

- **Powered by FactSage and ChemApp:** FactFlow employs the same thermodynamic equilibrium calculation algorithms and databases as FactSage and ChemApp, offering unparalleled accuracy.
- **Intuitive User Interface:** Designed to be user-friendly, FactFlow features a drag and drop flowsheet-based interface for process simulation.
- **Flexible Simulation Capabilities:** FactFlow supports a wide range of applications, from basic equilibrium calculations performed in series to complex process optimizations, steady-state simulations and parametric studies.
- **Comprehensive Analysis Tools:** FactFlow is equipped with extensive analysis and visualization tools, enabling users to experiment with different input parameters and allowing in-depth examination of results.
- **Long-term continuous development and support:** FactFlow is backed by a dedicated development team, ensuring regular updates, feature enhancements, and user support.



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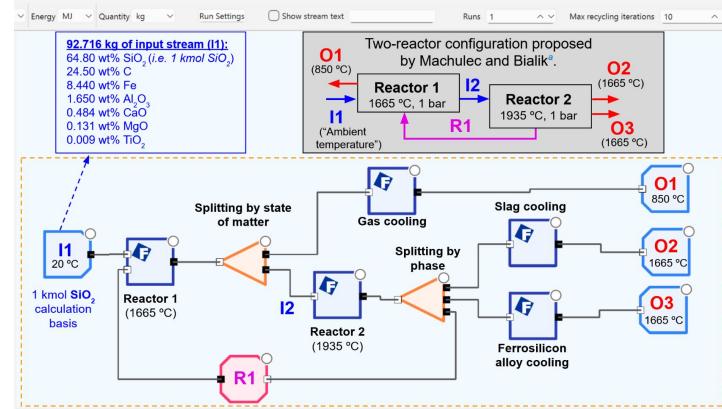
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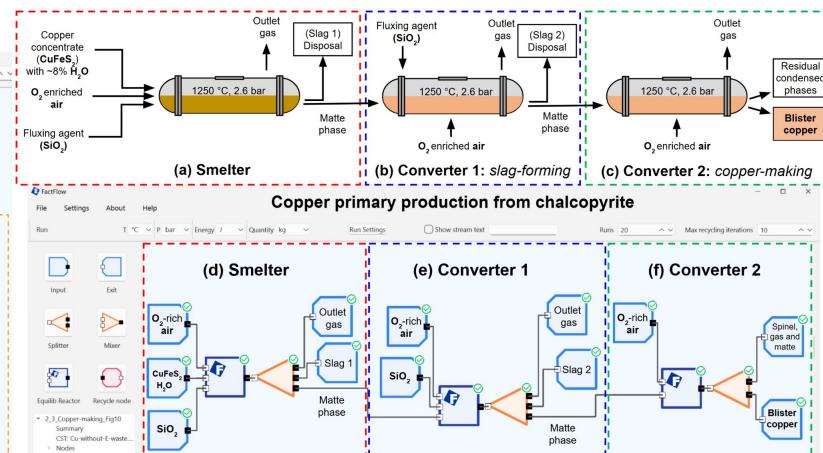
# What is FactFlow?

**FactFlow** has already been employed to model various processes, and has been used by industry partners around the world.

We have published a paper titled **Pyrometallurgical process modeling using FactFlow** in the *Calphad* journal that demonstrates FactFlow's capabilities through 4 examples of pyrometallurgical processes:



Ferrosilicon alloy production



Copper primary production



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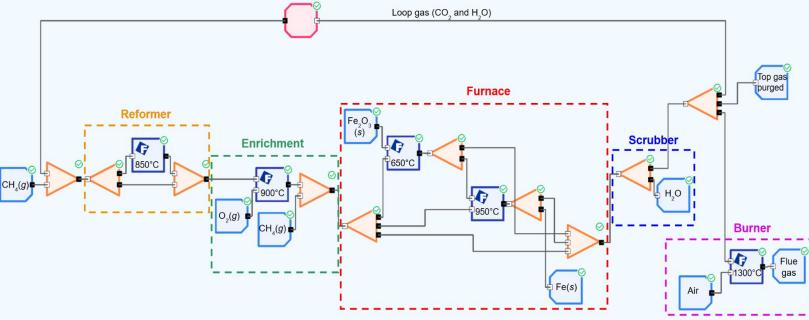
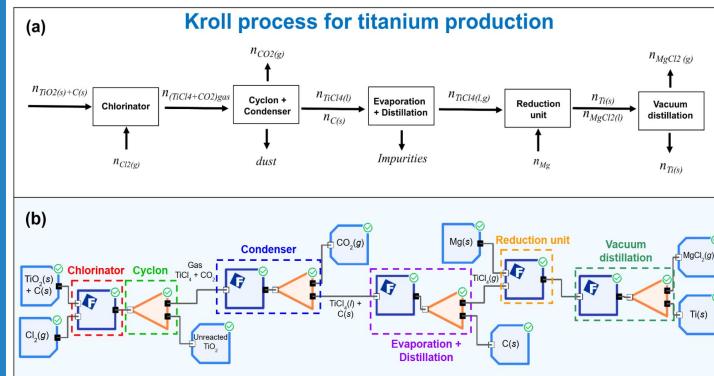
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MIDREX direct iron reduction process



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# About This Manual

This manual is designed to help you learn how to use FactFlow effectively, whether you're new or looking to explore more advanced features.

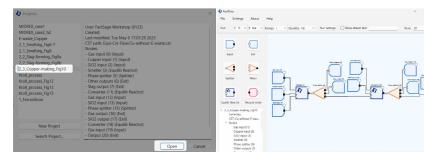
We strongly recommend beginning with the **Getting Started** section. It's a guided walkthrough that shows you how to **reproduce a real figure** from the FactFlow paper, step by step.

You'll follow along directly in your own FactFlow installation and learn how to:

- Launch FactFlow
- Open an example project
- Navigate the interface
- Run a calculation
- View and plot simulation results

This hands-on approach is the fastest way to become familiar with FactFlow's core workflow.

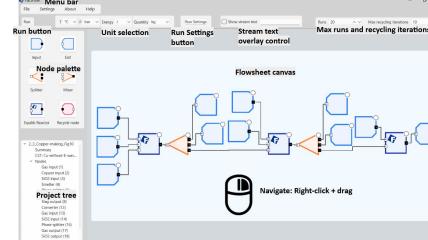
Getting Started - Open an example



FactFlow examples are a great way to learn how the software works and explore its capabilities. To open an example, select it from the list and click **Open** in the bottom-right corner.

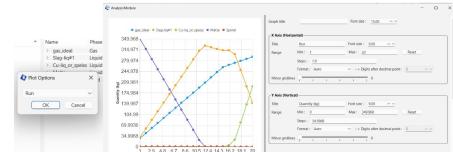
Try opening the **2\_3\_Copper-making\_Fig10** example. This example reproduces Figure 10 from Section 3.2.3 of the FactFlow paper. In the following steps, we'll walk through how to generate the plot shown in that figure.

Getting Started - Main interface



Navigate: Right-click + drag

Getting Started - Plot the results



In the **Plot Options** dialog, simply **click OK**. This will launch the **Analysis Module**, FactFlow's dedicated environment for advanced analysis and visualization. Plot settings and customization options will be covered later in this guide.

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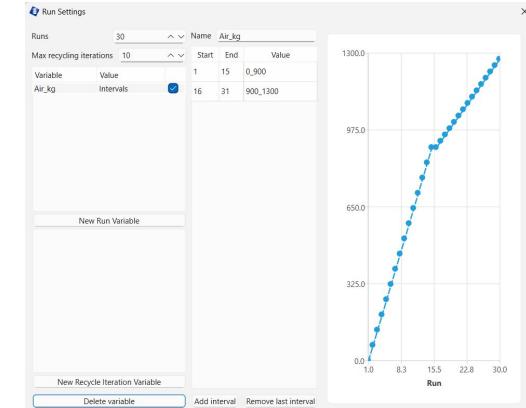
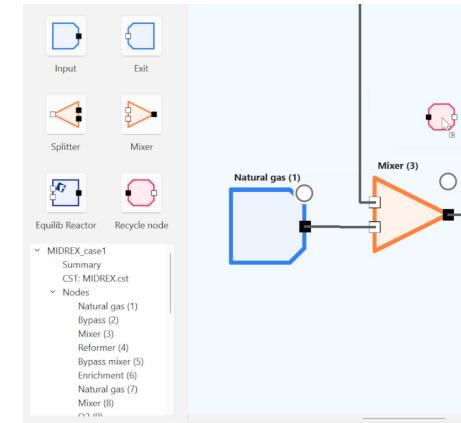
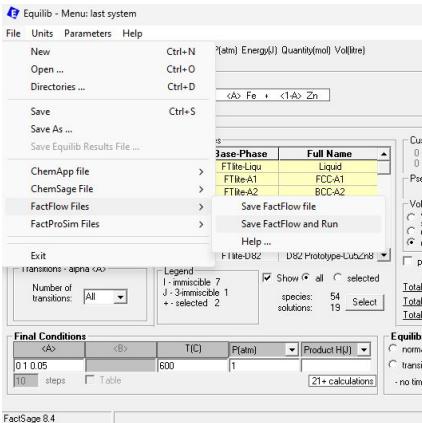
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# About This Manual

## What Comes Next - Creating your own Process Simulation

To create your own simulation, you'll follow a multi-step process. Each of these steps is explained in detail in this manual.



### Step 1

#### Prepare your Database

Use FactSage's Equilib module to perform the species and phase selection for your flowsheet's mini database.

### Step 2

#### Build the Process Flowsheet

Drag and connect nodes to model your process: inputs, reactors, splitters, recycling loops, etc.

### Step 3

#### Configure Run Settings

Define how many simulations to run and how input conditions should vary (e.g., temperature, quantity of reactants).



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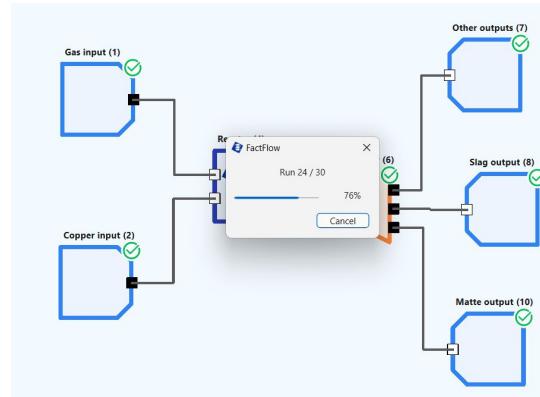
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# About This Manual

## What Comes Next - Creating your own Process Simulation

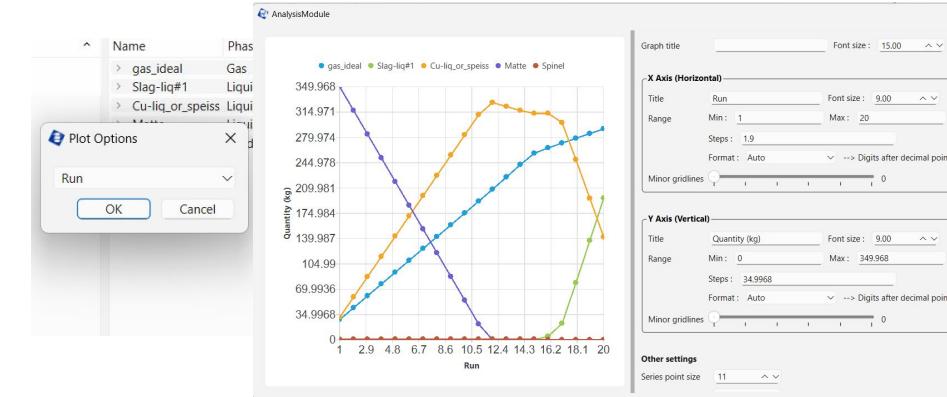
To create your own simulation, you'll follow a multi-step process. Each of these steps is explained in detail in this manual.



### Step 4

#### Run the Simulation

Launch the simulation—FactFlow will execute all runs, including parametric variations and recycle loops, progressing node by node until convergence.



### Step 5

#### Analyze the Results

Access calculation results from any node, then use the Analysis Module to plot trends, compare runs, or examine elemental compositions. You can also export data and plots for further use.



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# Getting Started

Now that you've seen the overall structure of the manual, it's time to get **hands-on**.

In this section, you'll reproduce a **real figure** from the FactFlow paper by following along with a **built-in example**.

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# Getting Started - System Requirements

Before launching FactFlow, make sure your system meets the following requirements:



- **Operating System:** Windows 10/11 or later
- **RAM:** 8GB minimum, 16GB recommended
- **FactSage Requirement:** Valid license of FactSage 8.4 or later



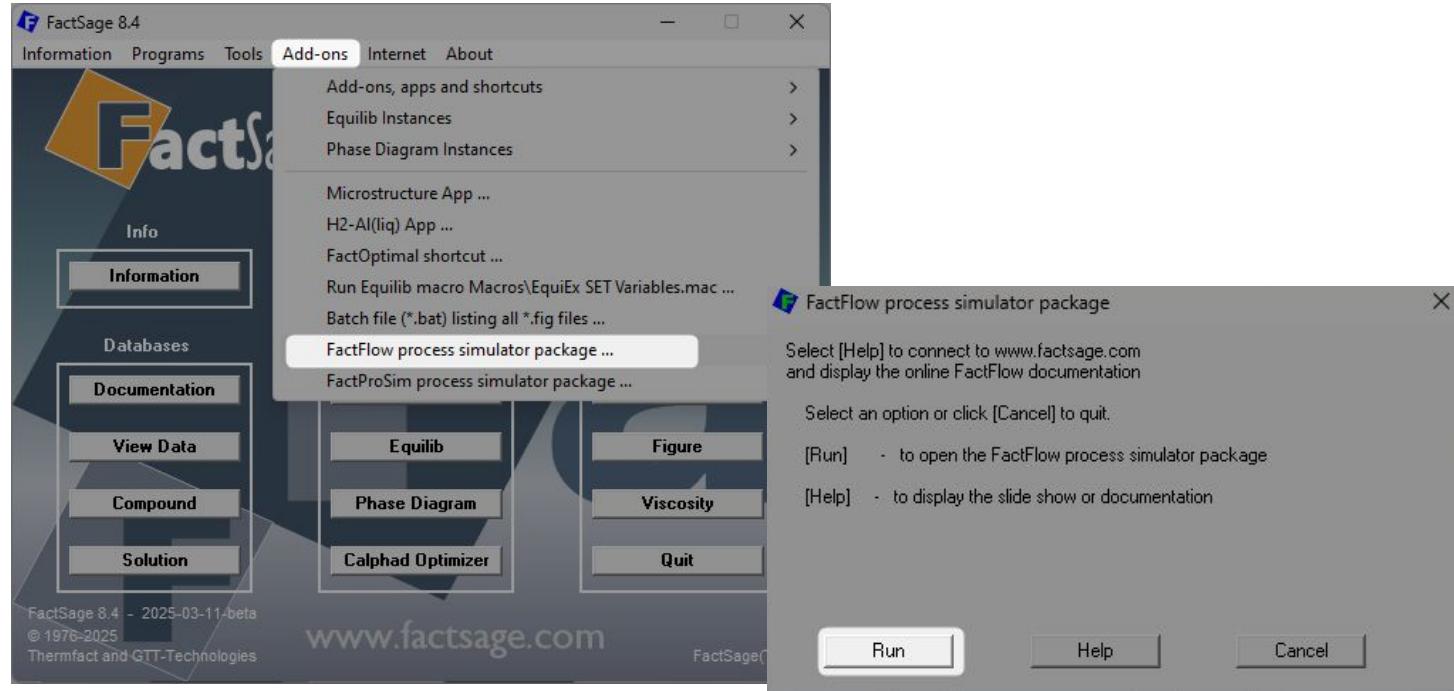
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# Getting Started - Launching FactFlow



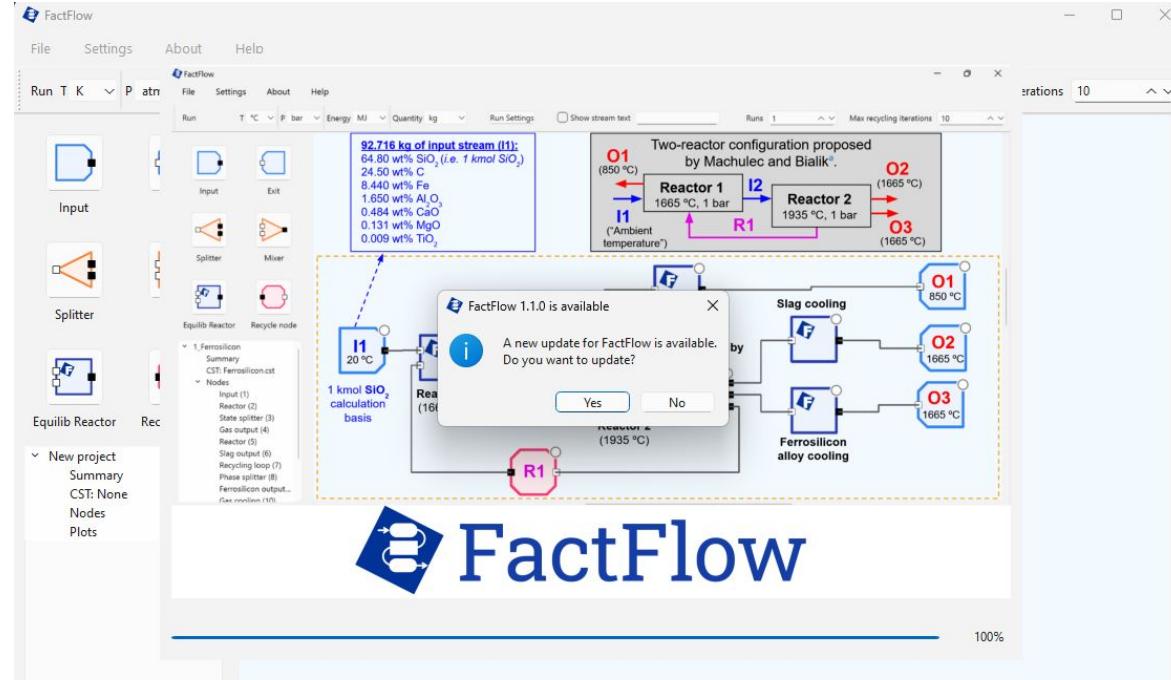
To launch FactFlow, open **FactSage**, then go to the **Add-ons** menu in the top toolbar and select **FactFlow process simulator package...** from the dropdown list. Click **Run** to launch FactFlow in the pop-up window.



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# Getting Started - Launching FactFlow



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On launch, FactFlow may prompt you to install an available update. We **highly recommend** clicking **Yes**—the update will run automatically, and FactFlow will relaunch once it's complete.



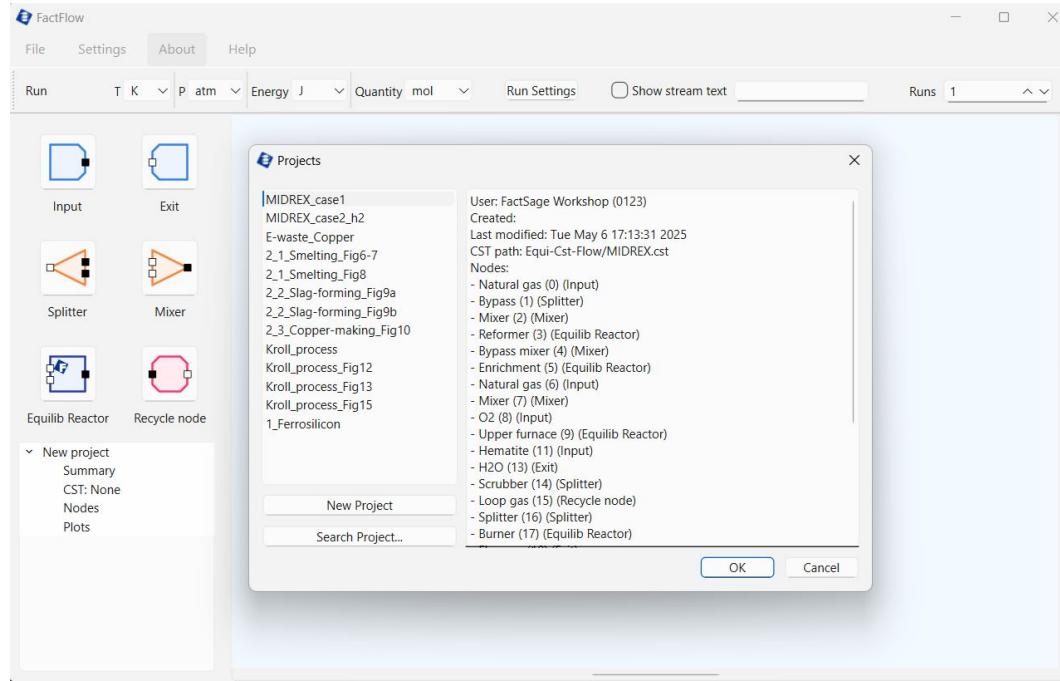
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# Getting Started - Projects window



Upon launch, FactFlow automatically opens the **Projects** window, where you can view, open, or create projects.



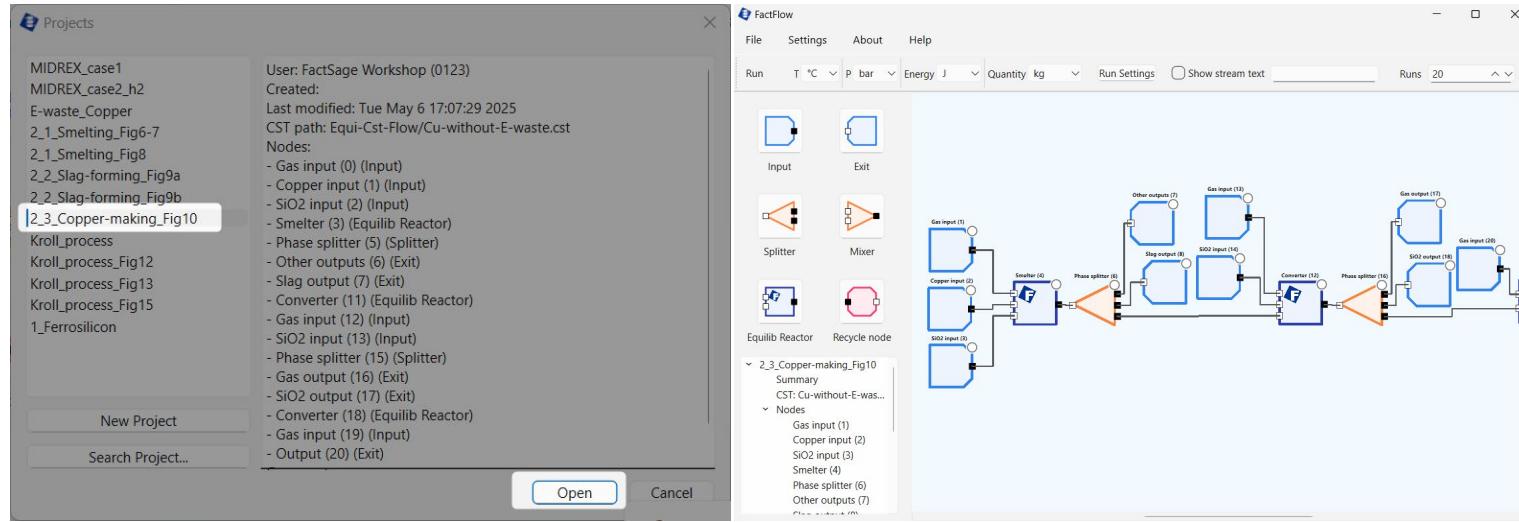
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# Getting Started - Open an example



**FactFlow examples** are a great way to learn how the software works and explore its capabilities. To open an example, select it from the list and click **Open** in the bottom-right corner.

Try opening the **2\_3\_Copper-making\_Fig10** example. This example reproduces Figure 10 from Section 3.2.3 of the FactFlow paper. In the following steps, we'll walk through how to generate the plot shown in that figure.



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# Getting Started - Main interface

FactFlow Main interface screenshot illustrating the Flowsheet canvas and various controls.

**Run button**: Located in the top left of the menu bar.

**Unit selection**: Located in the top center of the menu bar.

**Run Settings button**: Located in the top center of the menu bar.

**Show stream text**: Located in the top center of the menu bar.

**Stream text overlay control**: Located in the top right of the menu bar.

**Max runs and recycling iterations**: Located in the top right of the menu bar.

**Node palette**: Contains icons for Input, Exit, Splitter, Mixer, Equilib Reactor, and Recycle node.

**Flowsheet canvas**: The main workspace where the flowsheet diagram is displayed. It shows a complex network of blue lines representing streams and black nodes representing unit operations. Three orange nodes labeled 'F' are highlighted.

**Project tree**: Located in the bottom left of the interface, listing nodes and outputs:

- 2\_3\_Copper-making\_Fig10
- Summary
- CST: Cu-without-E-was...
- Nodes
  - Gas input (1)
  - Copper input (2)
  - SiO<sub>2</sub> input (3)
  - Smelter (4)
- Outputs
  - Slag output (8)
  - Converter (12)
  - Gas input (13)
  - SiO<sub>2</sub> input (14)
  - Phase splitter (16)
  - Gas output (17)
  - SiO<sub>2</sub> output (18)
  - Converter (19)

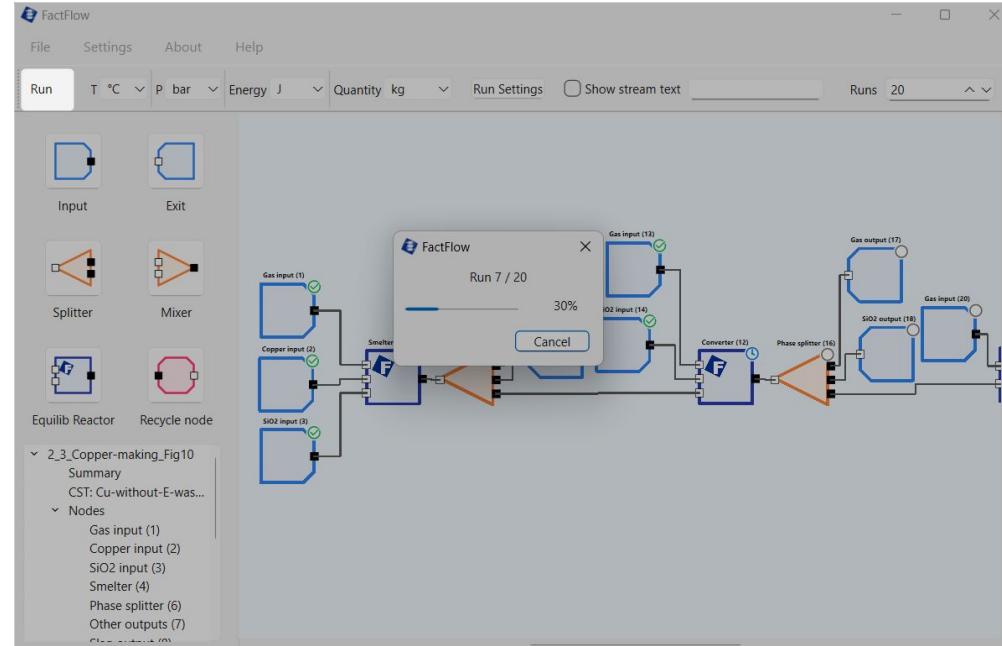
**Mouse cursor icon**: A large mouse cursor icon with a 'I' symbol, indicating a tooltip or help message.

**Navigate: Right-click + drag**: A text label indicating the navigation method for the Flowsheet canvas.



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Let's run the example. Click the **Run** button at the top left and wait for the simulation to complete. This example is set up to perform **20 runs, varying the amount of O<sub>2</sub>-enriched air input** in the second converter. You'll learn how to build your own flowsheet and configure runs later in the guide.



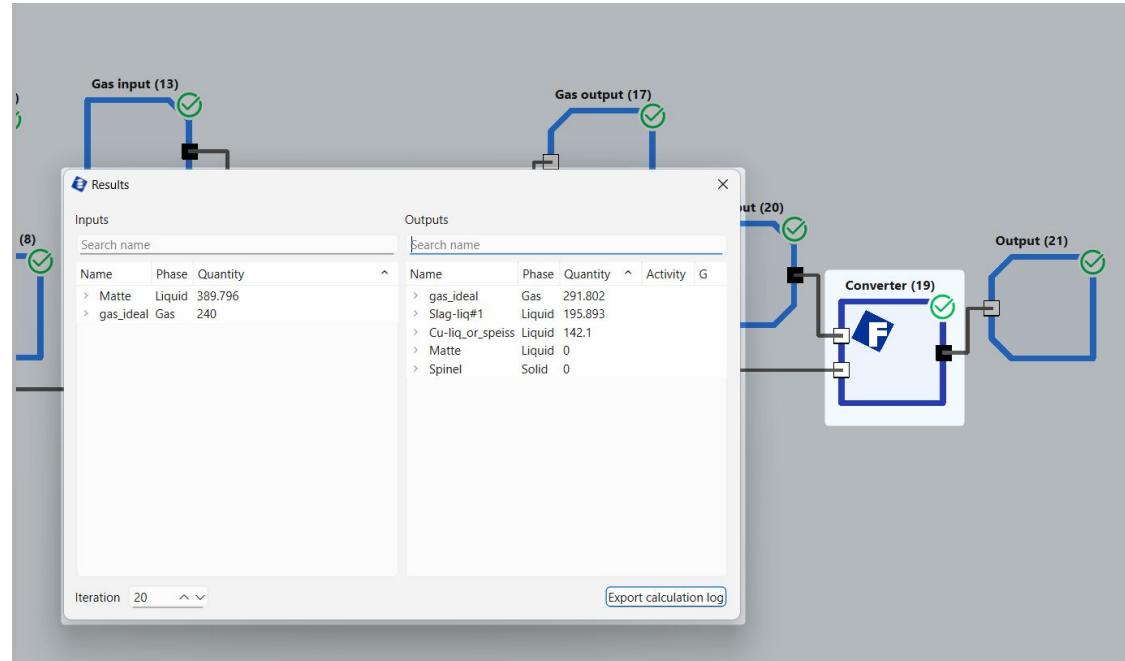
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# Getting Started - Plot the results



Once the calculation is complete, **right-click and drag to navigate** to the end of the flowsheet on the right. There, you'll find the **second converter**, modeled as an **Equilib Reactor node** labeled **Converter (19)**. **Double-click** this node to open its **Results** window.

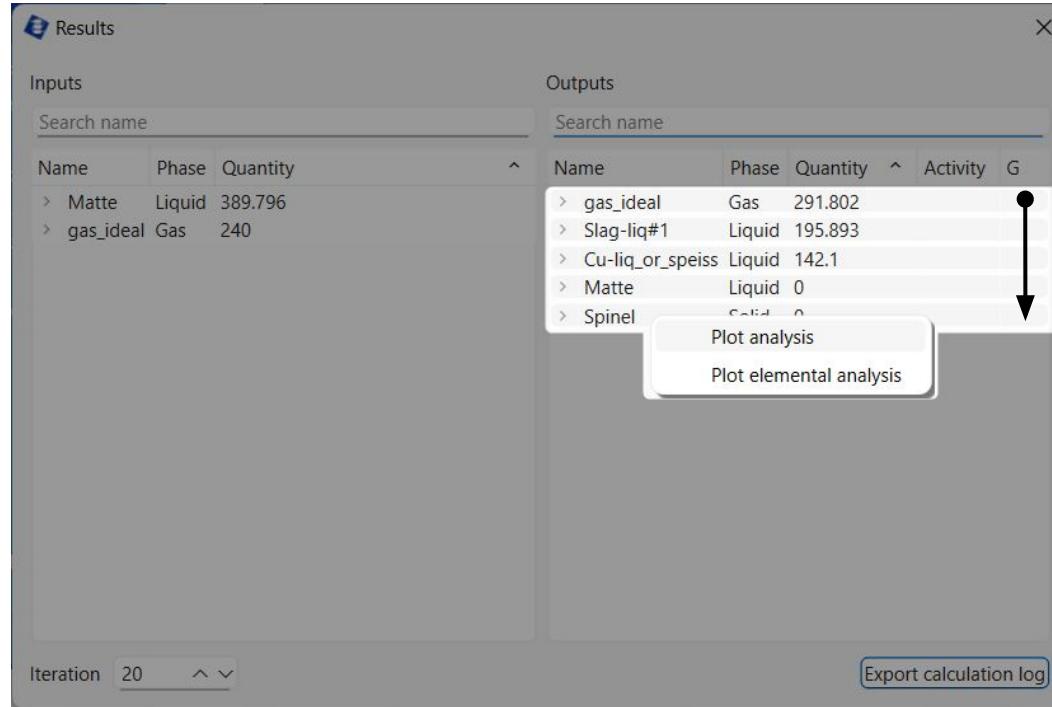
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# Getting Started - Plot the results



The screenshot shows the FactFlow software interface with the 'Results' window open. The 'Inputs' section lists two entries: 'Matte' (Liquid, 389.796) and 'gas\_ideal' (Gas, 240). The 'Outputs' section lists five phases: 'gas\_ideal' (Gas), 'Slag-liq#1' (Liquid), 'Cu-liq\_or\_speiss' (Liquid), 'Matte' (Liquid), and 'Spinel' (Solid). A context menu is open over the 'Outputs' section, with 'Plot analysis' and 'Plot elemental analysis' options highlighted.



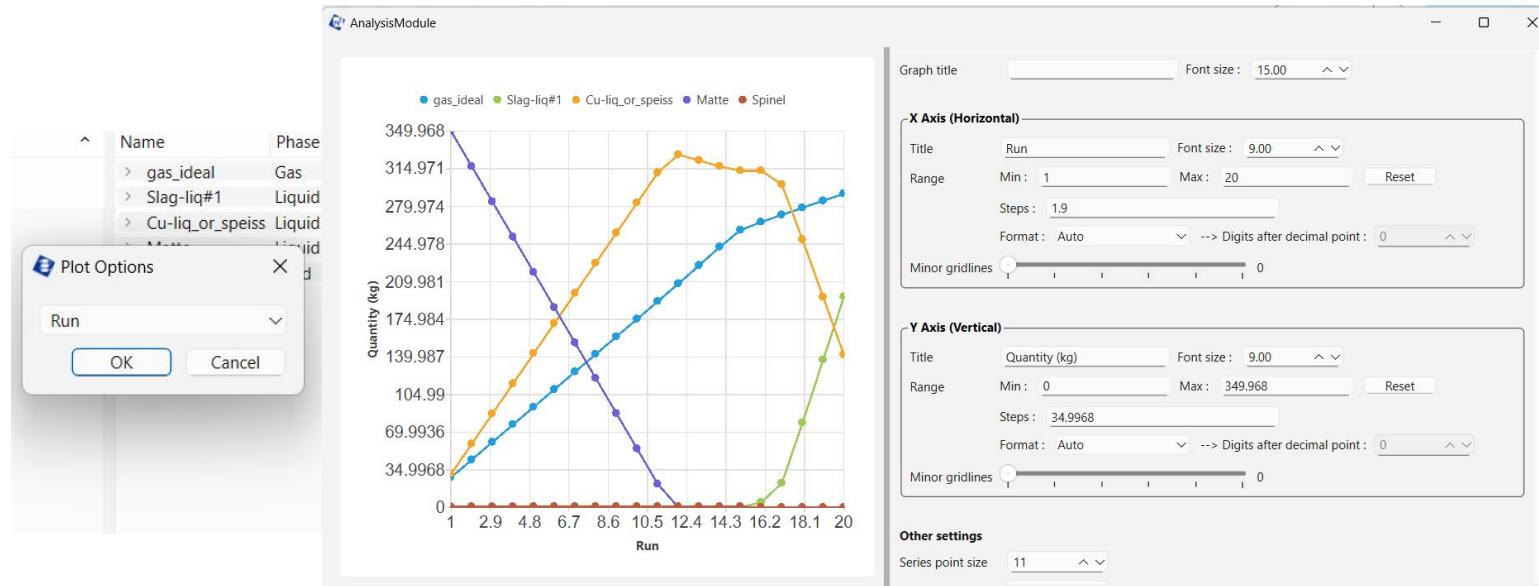
Multi-select: Left-click + drag

To select all phases in the **Outputs** section, click the first phase, then **hold left-click and drag down to the last one**. Alternatively, you can select individual phases by holding **Ctrl** and **left-clicking each**. Once all desired phases are selected, **right-click** and choose **Plot Analysis** to generate the plot.

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# Getting Started - Plot the results



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In the **Plot Options** dialog, simply click **OK**. This will launch the **Analysis Module**, FactFlow's dedicated environment for advanced analysis and visualization. Plot settings and customization options will be covered later in this guide.

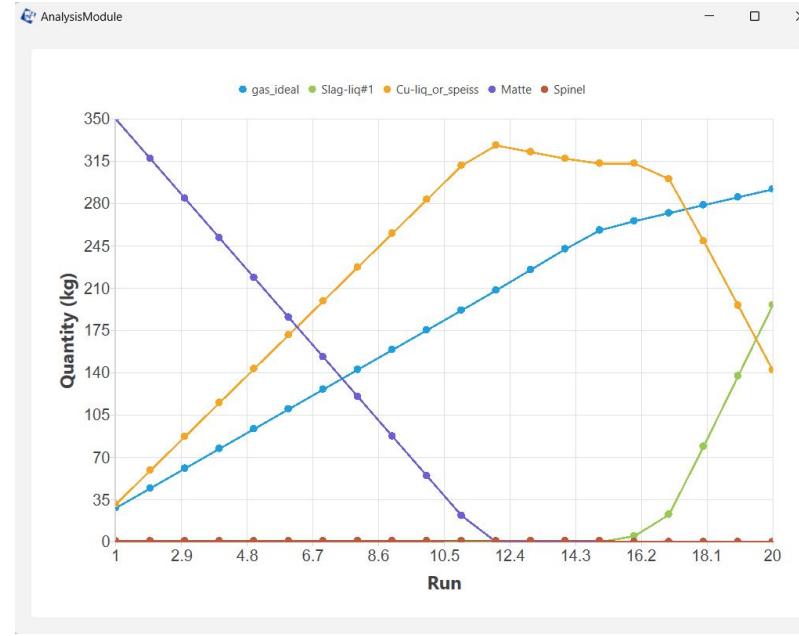
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# Getting Started - Plot the results



K. Poëti et al.

(a)

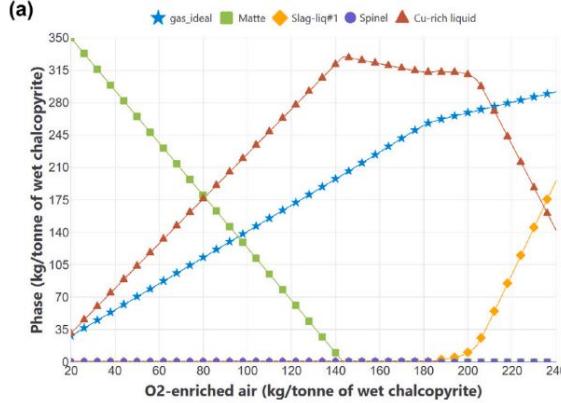


Fig. 10. (a) Phase assemblage evolution during the copper-making step (converter 2) as a function of the air injection in converter 2.

🎉 Congratulations! You've successfully reproduced **Figure 10a** from the **FactFlow paper**. Most figures in the paper were generated directly using the **Analysis Module**, and you'll find a corresponding **FactFlow example** for nearly every one. Feel free to explore them to deepen your understanding.  
<https://doi.org/10.1016/j.calphad.2024.102772>



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# Prepare your Database

Now that you've completed the guided example, it's time to **build your own simulation from scratch.**

The first step is to define the **chemical system** your process will use.

You'll do this using **FactSage's Equilib module**, which lets you select the relevant elements, species, and phases — and send them directly to FactFlow with a single click.

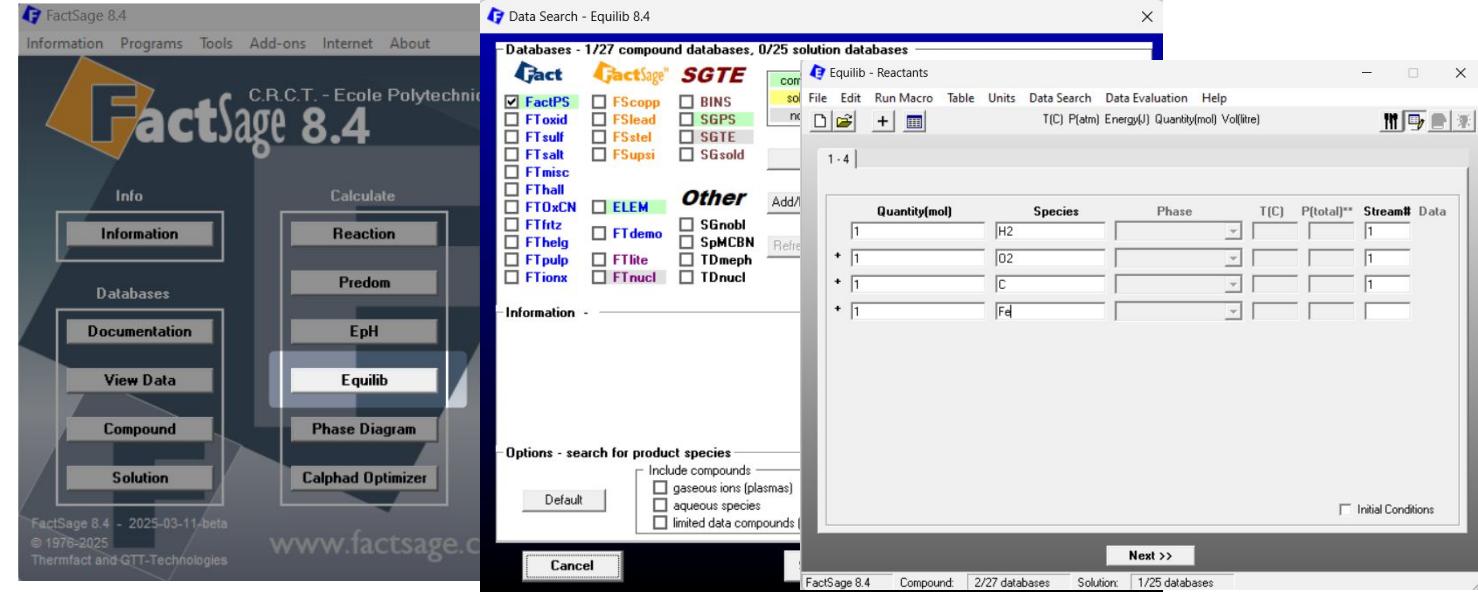
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# Prepare your Database



The screenshot shows the FactSage 8.4 software interface. On the left, the main menu bar includes Information, Programs, Tools, Add-ons, Internet, and About. Below the menu is a navigation bar with links to Info, Calculate, Databases, Documentation, View Data, Compound, and Solution. The Calculate section contains buttons for Reaction, Predom, EpH, Equilib, Phase Diagram, and Calphad Optimizer. The Databases section lists FactPS, FToxid, FTfull, FTsalt, FTmisc, FTHall, FTOxCN, FTfritz, FTHelg, FTpulp, and FTionx. The right side of the interface shows the Data Search - Equilib 8.4 dialog box. This dialog has tabs for 'Equilib - Reactants' and 'Other'. Under 'Other', there are checkboxes for BINS, SGPS, SGTE, SGsold, ELEM, FTdemo, SGNobi, SpMCBN, TDmeph, and TDnuc. The main area of the dialog box displays a table for inputting species and their quantities. The table has columns for 'Quantity(mol)', 'Species', 'Phase', 'T(C)', 'P[total]\*\*', and 'Stream#'. The first row shows H<sub>2</sub> at 1 mol. Below the table are options for searching product species, including checkboxes for 'Include compounds' (gaseous ions (plasmas), aqueous species, limited data compounds), a 'Default' button, and a 'Cancel' button. At the bottom right is a 'Next >>' button.

1. Launch the **Equilib module** in FactSage.
2. **Select the appropriate databases** in the Data Search menu.
3. **Enter the input species involved in your system.** The quantities can be arbitrary — they do not affect the mini-database used by FactFlow.

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# Prepare your Database

The screenshot shows the Equilib software interface. At the top, there's a menu bar with File, Units, Parameters, and Help. Below the menu is a toolbar with icons for opening files, saving, and other functions. A status bar at the bottom indicates "FactSage 8.4".

**Reactants (4)**

H<sub>2</sub> + O<sub>2</sub> + C + Fe

**Products**

Compound species

|                      |              |                                        |                            |    |
|----------------------|--------------|----------------------------------------|----------------------------|----|
| [+]                  | gas          | <input checked="" type="radio"/> ideal | <input type="radio"/> real | 45 |
| [+]                  | aqueous      | 0                                      |                            |    |
| [+]                  | pure liquids | 0                                      |                            |    |
| * [+]                | pure solids  | 26                                     |                            |    |
| * - custom selection |              | species: 71                            |                            |    |

Target  
- none -  
Estimate T(K): 1000  
Quantity(mol): 0

**Solution phases**

|   | Base-Phase  | Full Name           |
|---|-------------|---------------------|
| I | FTlite-Liqu | Liquid              |
| J | FTlite-A1   | FCC-A1              |
| I | FTlite-A2   | BCC-A2              |
| I | FTlite-A3   | HCP-A3              |
| I | FTlite-A4   | DIAM-A4 Prototype-C |
| I | FTlite-C14  | C14 Prototype-MgZn2 |

Legend  
I - immiscible 5  
J - 3-immiscible 1  
 Show all  selected  
species: 44 Select  
solutions: 13 Select

**Custom Solutions**  
0 fixed activities Details...  
0 ideal solutions

**Pseudonyms**  
apply  Edit...

Volume and physical prop data  
 assume molar volumes of solids and liquids = 0  
 use only molar volume data  
 use V & phys. property data

paraequilibrium & Gmin edit

Total Species (max 7000) 115  
Total Solutions (max 200) 13  
Total Phases (max 1500) 40

**Equilibrium**  
 normal  normal + transitions  
 transitions only  open  
- no time limit - **Calculate >**

**Perform the phase selection** by choosing all phases that may form in your system. This ensures the generated database includes all relevant phase data.

Temperature, pressure, and other calculation conditions do not affect the database generation and can be left unchanged.



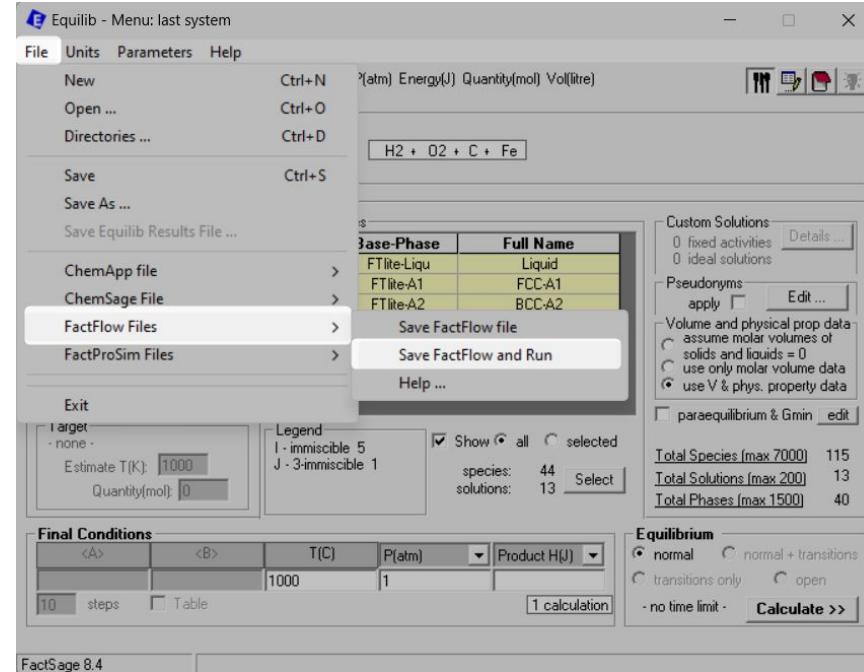
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# Prepare your Database



Send your system to FactFlow by selecting **File → FactFlow Files → Save FactFlow and Run**.

This generates the mini database in the background and automatically launches FactFlow with your selected system.



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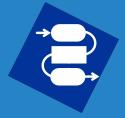
# Prepare your Database – Behind the scenes

When you select **Save FactFlow and Run** in the **Equilib** module, FactFlow prepares and stores the files needed for your simulation.

Here's what happens behind the scenes:

- All project files are saved directly inside the **Equi-Cst-Flow** folder in the FactFlow directory. This is the central location where all FactFlow projects are kept.
- Three files are created for your project:
  - **.equi** file – Describes the equilibrium system prepared in Equilib
  - **.cst** file – A compiled binary file representing the mini database (This is what FactFlow actually uses during calculations)
  - **.flow** file – Stores the flowsheet, node configurations, and simulation settings

These files work together to define and run your simulation — there's no need to manage them manually, but it's helpful to understand how they relate.



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# Build the Flowsheet

Now that FactFlow is launched with your system, it's time to **build your process flowsheet**.

In this section, you'll learn how to model your process using **nodes** — the building blocks of a simulation. You'll place, connect, and configure nodes to represent **inputs, reactors, splitters, outputs, and recycling loops**, forming the structure of your simulation.

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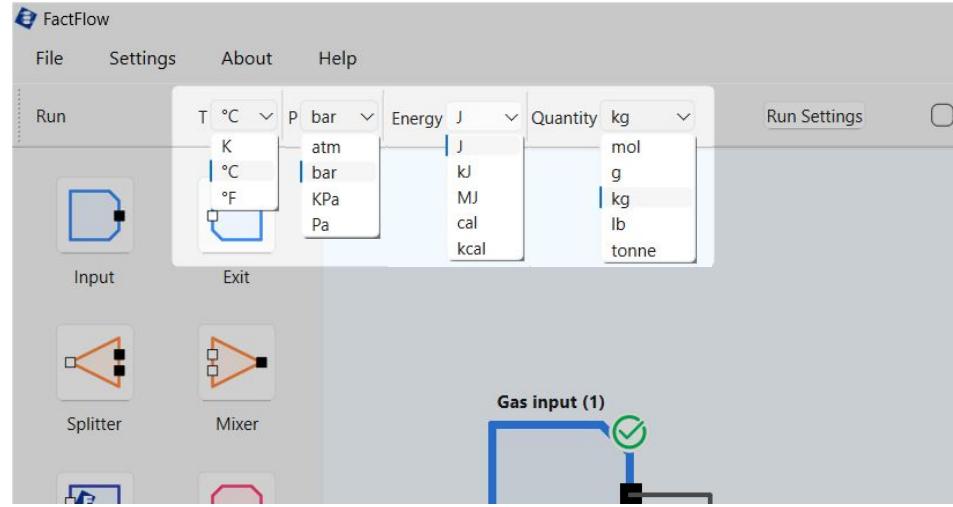
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# Build the Flowsheet - Units selection



Before building your flowsheet, **choose the units you'd like to work with**. Use the dropdown menus at the top of the FactFlow window to select units for **temperature, pressure, energy, and quantity**.

You can change these units at any time — they only affect how values are displayed and entered in the interface.



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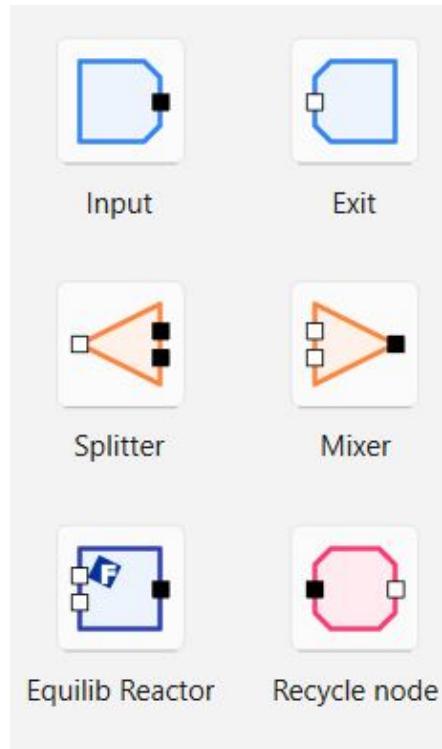
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# Build the Flowsheet - Node Types

FactFlow simulations are built using interconnected **nodes**, each representing a specific role in the process.



- **Input:** Defines an input stream, including phase or constituent quantities, as well as its temperature and pressure.
- **Exit:** Retrieves and displays the results of a given output stream for analysis.
- **Equilib Reactor:** Performs an equilibrium calculation using the same algorithm as FactSage.
- **Splitter:** Divides a stream based on flow rate, phase, or state.
- **Mixer:** Combines multiple input streams without performing an equilibrium calculation.
- **Recycle node:** Loops part of an output back into the system for iterative convergence.

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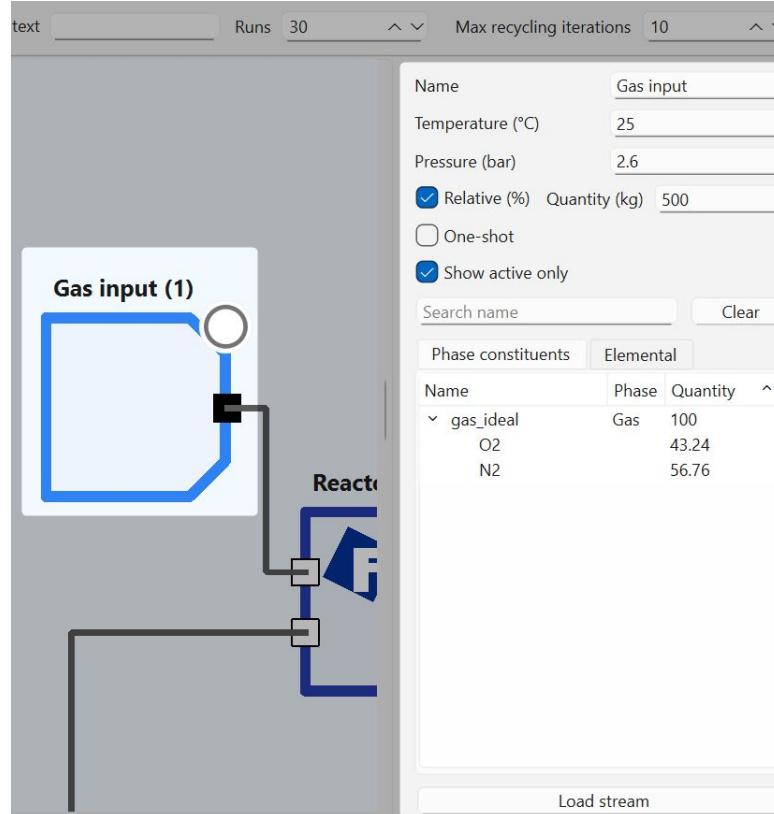
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# Build the Flowsheet - Input node

All nodes in FactFlow have an **Inspector**, which you can open by clicking on the node.



For the **Input** node, the Inspector allows you to:

- Set the **temperature** and **pressure** of the input stream
- Define the **stream composition** by entering phase or constituent quantities

You can use the **search box** to quickly locate species and the "**Show active only**" option to filter for non-zero entries.

Input nodes introduce material into the process and serve as entry points to the flowsheet.

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# Build the Flowsheet - Input node

You can define stream composition in two ways: using **absolute quantities** or **relative percentages**. Toggle between modes using the "**Relative (%)**" checkbox in the Input node Inspector.

## Absolute entry ("Relative (%)" is off, default)

- Double-click a cell in the **Quantity** column to enter a value
- Total amount is determined by what you input

| Name                   | Phase  | Quantity |
|------------------------|--------|----------|
| H2O_liquid(liq)        | Liquid | 80       |
| CuFeS2_Chalcopyrite(s) | Solid  | 920      |

## Relative entry ("Relative (%)" is checked)

- Enter percentage values in the Quantity column
- Total must equal 100

| Phase constituents |       |          |
|--------------------|-------|----------|
| Name               | Phase | Quantity |
| gas_ideal          | Gas   | 100      |
| O2                 |       | 43.24    |
| N2                 |       | 56.76    |

Relative (%)     Quantity (kg)

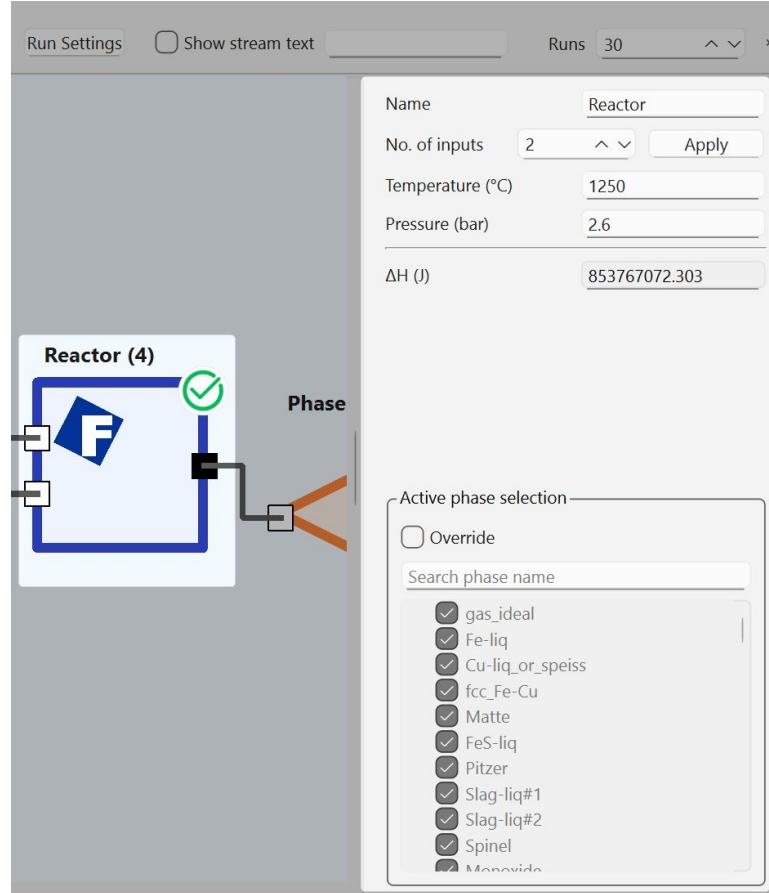
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# Build the Flowsheet - Equilib Reactor



The screenshot shows the FactFlow software interface. On the left, the Flowsheet builder displays a reactor node labeled "Reactor (4)" with an input stream labeled "F" and an output stream labeled "Phase". In the center, the Inspector panel is open for the reactor node. It contains the following settings:

|                  |               |
|------------------|---------------|
| Name             | Reactor       |
| No. of inputs    | 2             |
| Temperature (°C) | 1250          |
| Pressure (bar)   | 2.6           |
| ΔH (J)           | 853767072.303 |

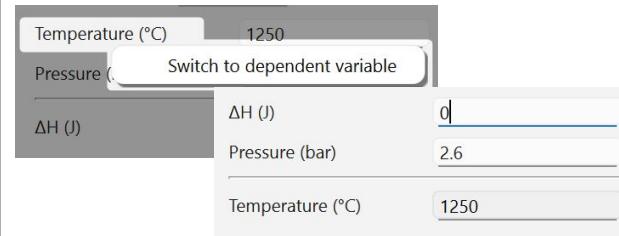
Below these settings is a section titled "Active phase selection" with a checkbox labeled "Override". A dropdown menu titled "Search phase name" lists various phases, with several checked:

- gas\_ideal
- Fe-liq
- Cu-liq\_or\_speiss
- fcc\_Fe-Cu
- Matte
- FeS-liq
- Pitzer
- Slag-liq#1
- Slag-liq#2
- Spinel
- Manganite

For the **Equilib Reactor** node, the Inspector allows you to:

- **Set any 2 of the following:** Temperature, Pressure, ΔH.
- **Number of inputs:** Set how many streams feed into this reactor.

To switch which variable is calculated, right-click on it and select “Set as dependent variable.”



To simulate an adiabatic reaction, set Temperature as the dependent variable and enter  $\Delta H = 0$ .



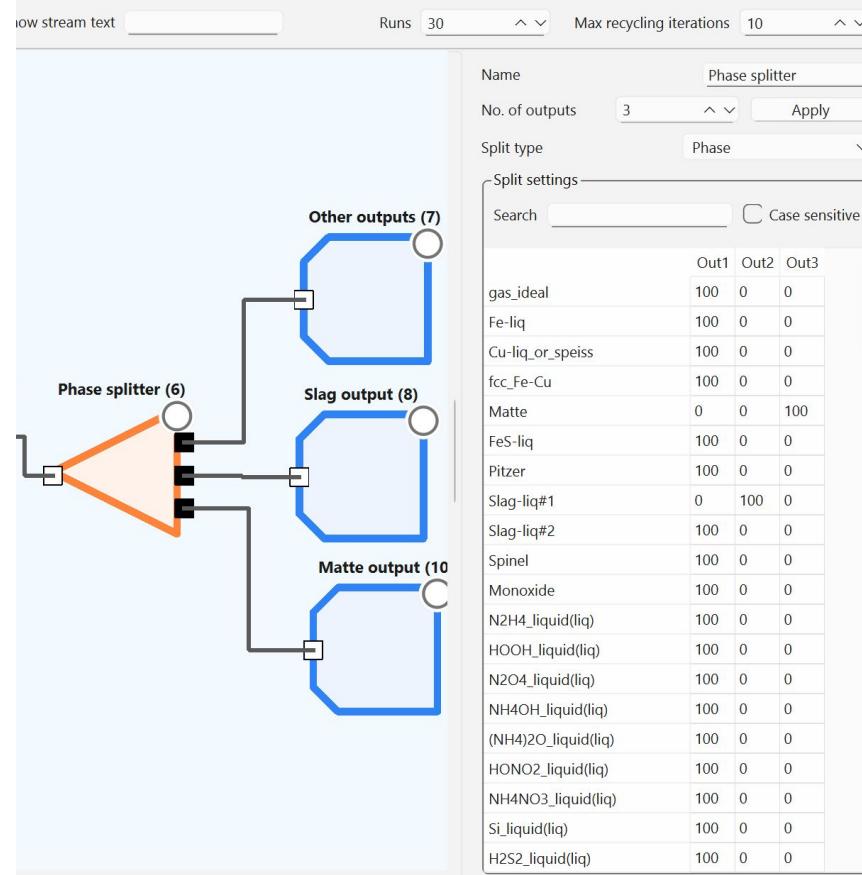
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# Build the Flowsheet - Splitter node



The **Splitter** node is used to divide an input stream into multiple output streams.

## **Split types:**

- **Flow:** Splits the entire stream by total flow percentage.
  - **Phase:** Splits the stream by phase (e.g., metal, slag, matte).
  - **State:** Splits by state of matter (solid, liquid, gas).

In all modes, percentages determine how much of each part of the stream is routed to each output.

Use Splitter nodes when directing specific parts of a stream to different process paths.

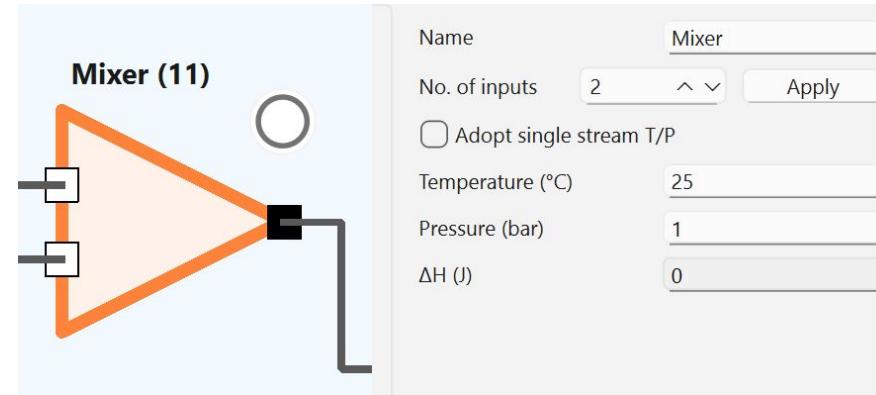
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# Build the Flowsheet - Mixer node

The **Mixer** node combines multiple input streams into a single output without performing an equilibrium calculation.



## Configuration

- **Number of inputs:** Set how many streams enter the Mixer.
- **Temperature & Pressure:** These values are imposed on the mixed stream.
- **ΔH:** Displays the energy required to bring all inputs to the target T/P.

**Adopt single stream T/P:** If this box is checked and **only one non-empty stream** enters the Mixer, the Mixer will:

- Ignore the user-specified T/P
- Adopt the temperature and pressure of that single stream

This is useful when using the Mixer as a **pass-through node** — nothing is altered unless multiple streams are present. When multiple streams are non-empty, the Mixer reverts to its standard behavior: mixing them and applying the defined T/P.



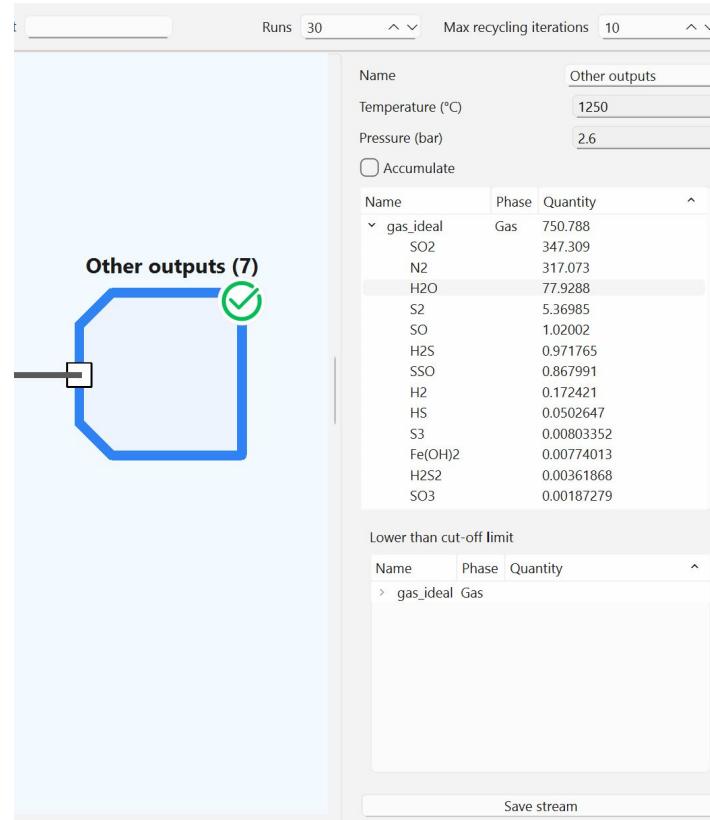
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# Build the Flowsheet - Exit node

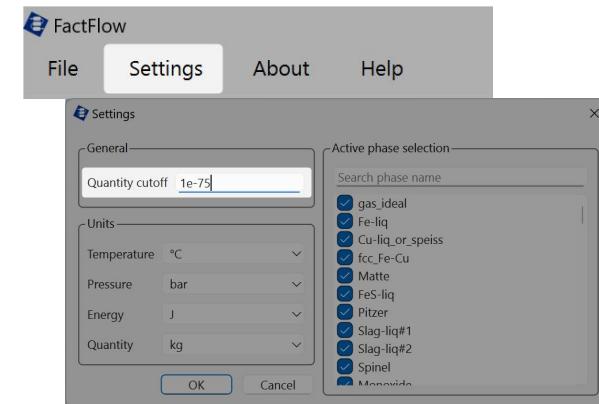
The **Exit** node is used to view the contents of an output stream in your flowsheet.



The Inspector lists all **phases and constituents**, along with their quantities.

Species below the cut-off limit appear in a separate section.

You can adjust the cut-off limit in Settings:



**Accumulate:** Sums output values across multiple recycling iterations.

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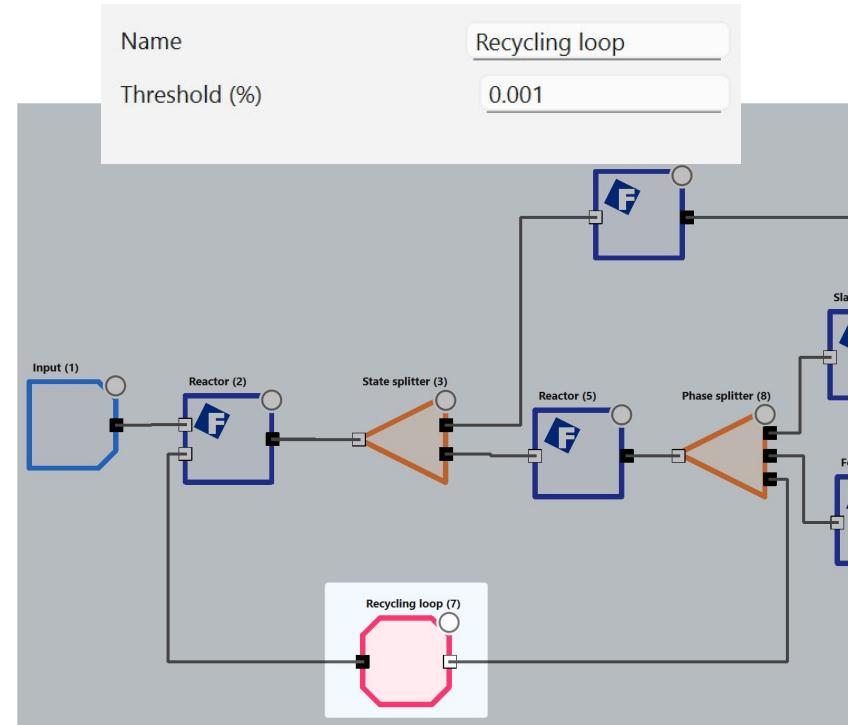
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# Build the Flowsheet - Recycle node

The **Recycle** node allows part of a stream to be sent back to an earlier point in the flowsheet, enabling **Recycling Iterations**.



The **Threshold (%)** setting controls when the recycling loop should stop.

For each phase or constituent, FactFlow checks whether the **percentage change** in quantity between two consecutive iterations is below the threshold.

The loop stops once **all values** meet this condition, or when the **maximum number of recycling iterations** is reached.

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



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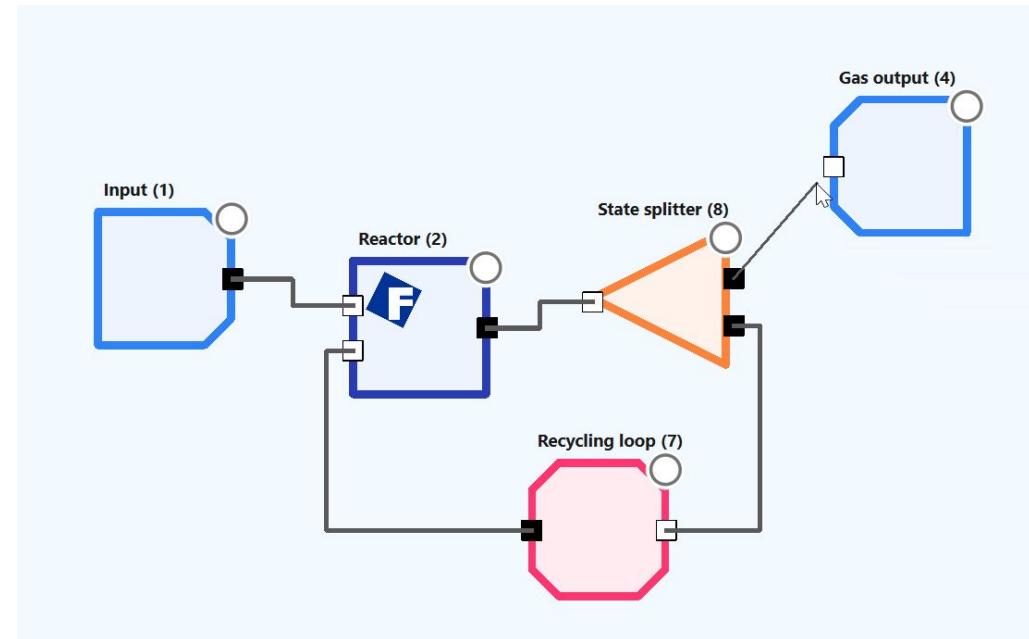


# Build the Flowsheet - Connecting nodes

To connect nodes:

- Click and drag from the **output port (black square)** of one node
- Drop the line onto the **input port (white square)** of the next node

You can combine nodes freely to represent your process flow.





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# Configure Run Settings

Now that your flowsheet is built, it's time to configure how the simulation will run.

In this section, you'll learn how to:

- Set how many **runs** to perform (e.g., for parametric studies)
- Set how many **recycling iterations** are allowed (if your flowsheet includes Recycle nodes)
- Vary **input conditions** across both runs and recycling iterations
- Use the **Run Settings panel** to assign variables and control simulation behavior



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# Configure Run Settings

## Understanding Runs vs. Recycling Iterations

When you run a simulation in FactFlow, there are **two layers** of calculation:

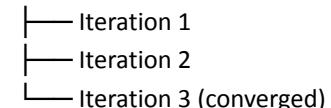
### 1. Runs (Parametric Runs)

- Each **Run** represents a **separate simulation** with a **unique set of input values**.
- You can vary inputs like temperature, reactant amount, or pressure across runs.
- Used to perform **parametric studies** and see how outputs change with different conditions.

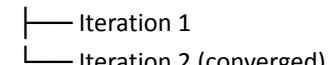
### 2. Recycling Iterations (Inside each Run)

- If your flowsheet includes a **Recycle node**, FactFlow will perform **multiple internal recycling iterations within each Run**.
- These iterations continue until:
  - All recycle loops converge (based on the threshold you set), or
  - The **Max recycling iterations** limit is reached.

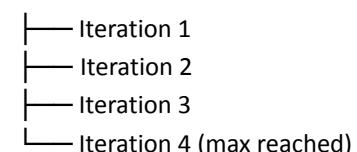
#### Run 1



#### Run 2



#### Run 3





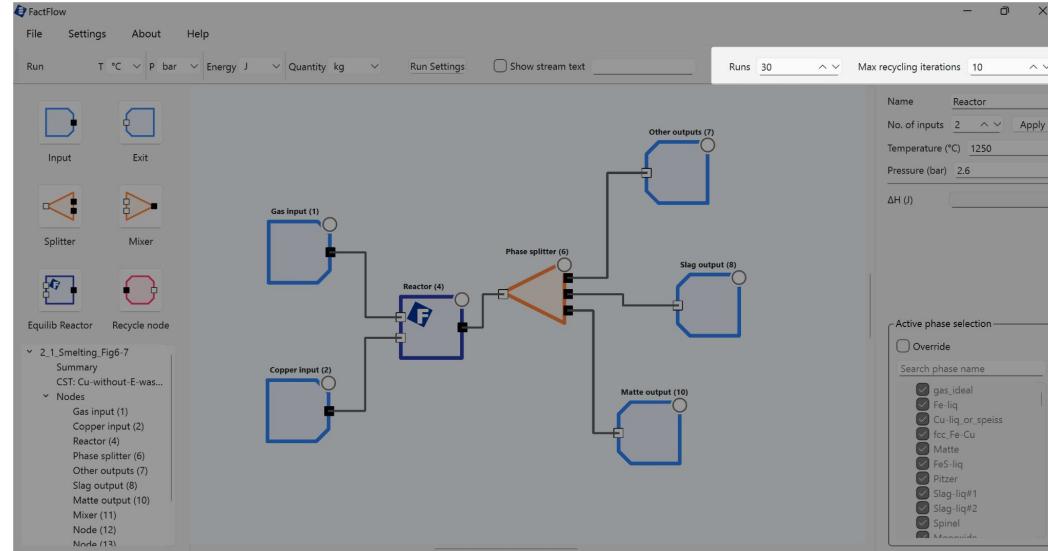
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# Configure Run Settings



## Set Runs and Max Recycling Iterations

- **Runs field:** Controls how many parametric runs will be executed.
- **Max recycling iterations field:** Controls the maximum number of iterations per run *if* recycling is active.

**Note:** In the example shown, there are no Recycle nodes in the flowsheet. Even though the Max recycling iterations is set to 10, no recycling will occur — only one calculation is performed per run.



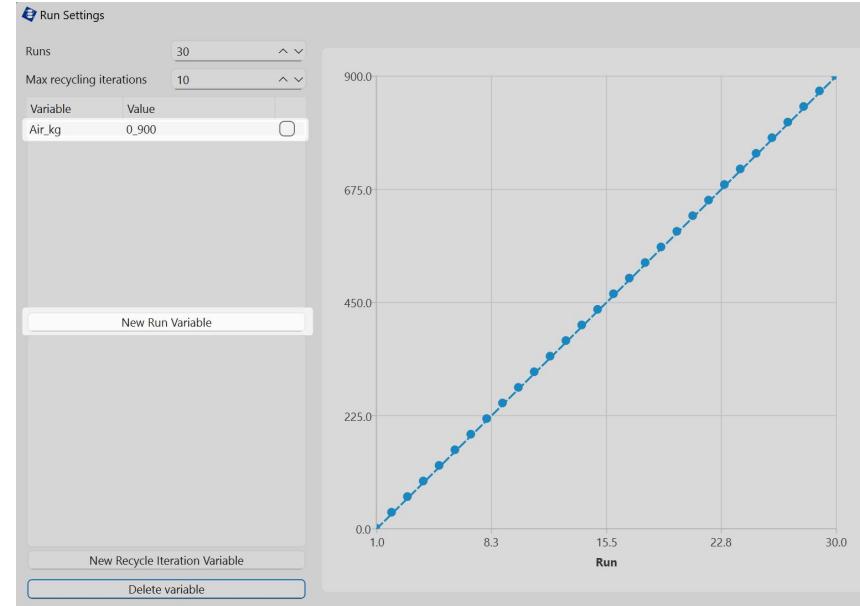
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# Configure Run Settings - Creating a Run Variable



- Click **New Run Variable** to add a variable.
- Enter the variable's name in the field that appears.
- Rename a variable at any time by double-clicking its name in the variable list.
- In the **Value** column, enter a range using the format: **MIN\_MAX**
  - Example: 0\_900 will vary the value from 0 to 900 across all runs.
  - Steps are automatically divided evenly.



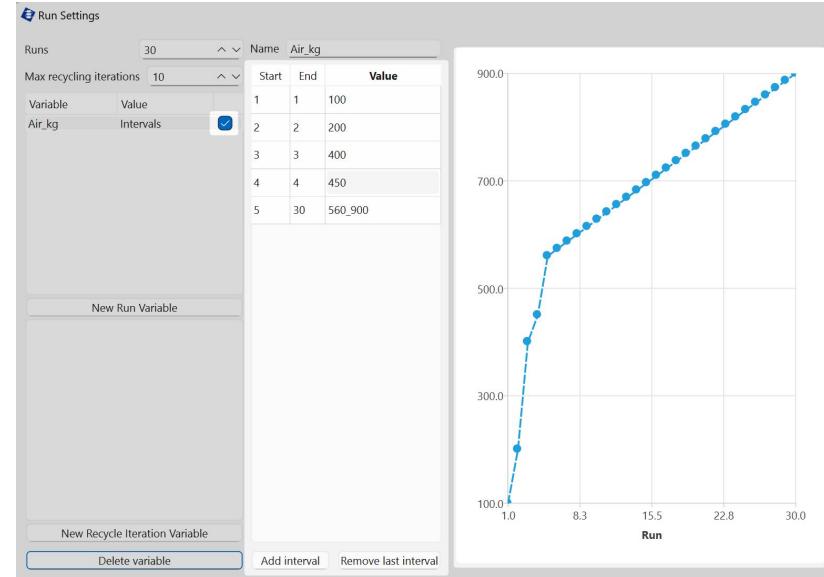
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# Configure Run Settings - Advanced Intervals



**Tip:** You can mix fixed values and ranges in the same variable. This is especially useful when working with multiple run variables, allowing you to keep one value constant while varying another.

- Check the box next to a variable to enable **Interval Mode**.
- This opens a table where you can define multiple **intervals**, each with:
  - A **Start** and **End** run index
  - A **Value**, which can be:
    - A **fixed value** (e.g., 400)
    - A **range** (e.g., 560\_900), which will be linearly interpolated across the interval
  - Use the **Add interval** and **Remove last interval** buttons to manage rows.



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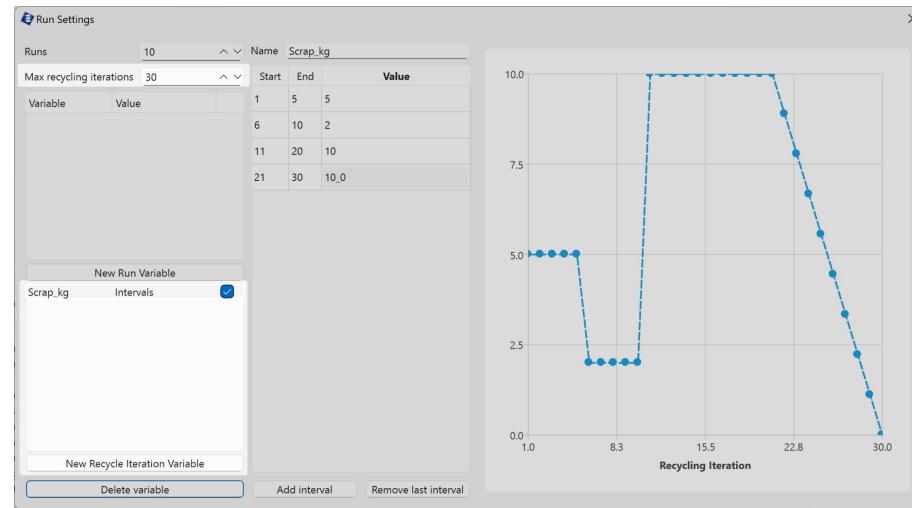
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# Configure Run Settings - Recycle Iteration Variables (Advanced)

Most simulations vary input values across runs, but you can also vary inputs **within each run**, across **recycling iterations**. This feature is especially useful for modeling **parameterized behaviour as a function of the recycling iteration**.



How to Define One:

- Click **New Recycle Iteration Variable** in the Run Settings panel.
- Enter the variable name and range (MIN\_MAX) just like a Run Variable.
- Optionally, enable **Interval Mode** for finer control across iterations.



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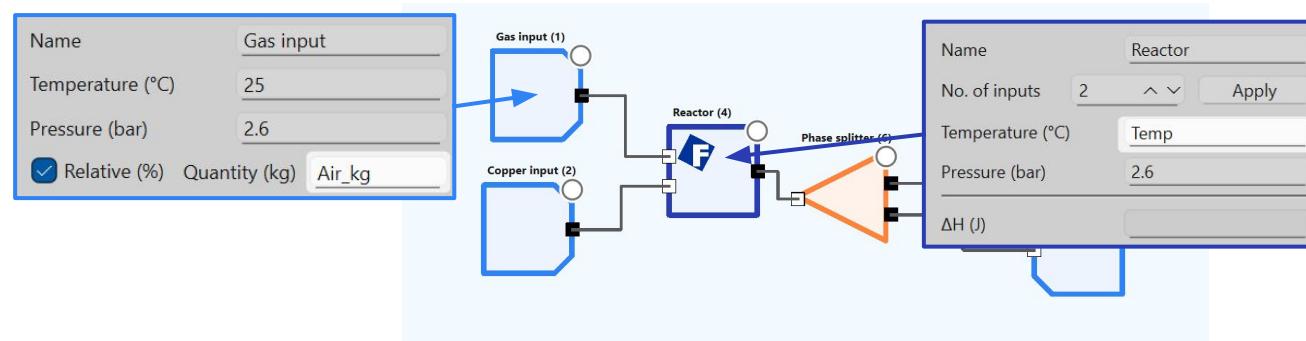


# Configure Run Settings - Using Variables in the Flowsheet

To use a **Run Variable** or **Recycle Iteration Variable**, simply type the variable's name into any **editable input field** in your flowsheet.

You can use variables in:

- **Temperature or Pressure** fields of Equilib Reactors
- **Quantities** in Input nodes
- **Percentage splits** in Splitter nodes (*more advanced — covered later in the Function Builder section*)



FactFlow will automatically substitute the correct value for each run or iteration based on your definitions in the **Run Settings** panel.

**Tip:** You can use multiple variables in a single simulation to explore combinations of process conditions.



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# Configure Run Settings - Importing Variables from Excel

You can define **Run Variables** and **Recycle Iteration Variables** by importing them from an Excel file.

- The **first sheet** in the Excel file is used to define variables that vary across **runs**
- The **second sheet**, if present, is used to define variables that vary across **recycling iterations**
- If only one sheet is included, FactFlow will assume it defines **Run Variables**

Each column defines a **separate variable**, and each row provides the value for a specific run or iteration (starting from 1).

|    | A    | B |
|----|------|---|
| 1  | Temp |   |
| 2  | 100  |   |
| 3  | 200  |   |
| 4  | 300  |   |
| 5  | 400  |   |
| 6  | 500  |   |
| 7  | 600  |   |
| 8  | 700  |   |
| 9  | 800  |   |
| 10 | 900  |   |
| 11 | 1000 |   |
| 12 | 1100 |   |
| 13 | 1200 |   |
| 14 | 1300 |   |
| 15 | 1400 |   |
| 16 | 1500 |   |
| 17 |      |   |

|    | A      | B      |
|----|--------|--------|
| 1  | O2_mol | Purity |
| 2  | 1      | 50     |
| 3  | 2      | 50     |
| 4  | 3      | 50     |
| 5  | 4      | 50     |
| 6  | 5      | 50     |
| 7  | 6      | 80     |
| 8  | 7      | 80     |
| 9  | 8      | 80     |
| 10 | 9      | 80     |
| 11 | 10     | 80     |
| 12 | 11     | 80     |
| 13 | 12     | 80     |
| 14 | 13     | 80     |
| 15 | 14     | 80     |
| 16 | 15     | 80     |
| 17 |        |        |



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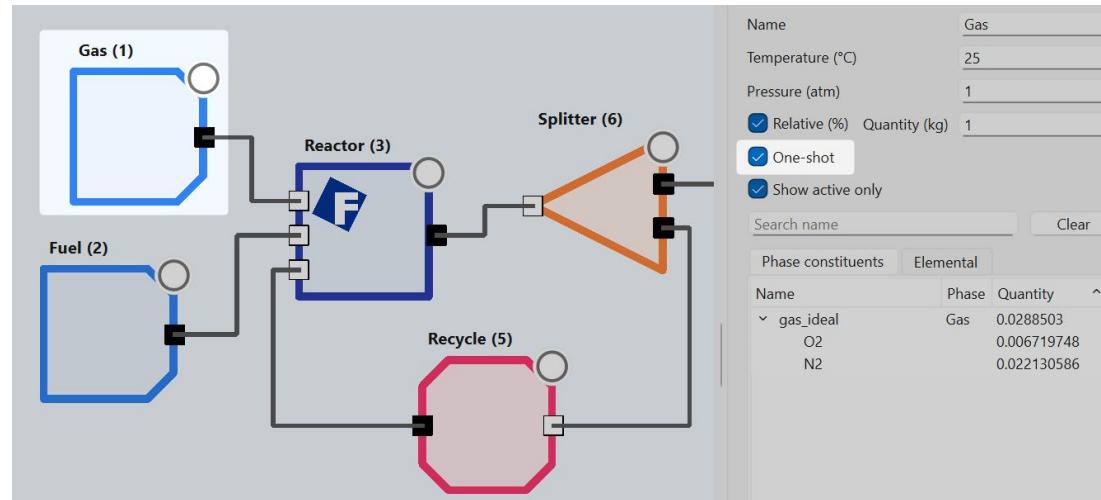


# Configure Run Settings - One-shot Input nodes

In flowsheets with recycling, some inputs may only be intended to act **once**, such as an initial dose of fuel, gas, or a reactant.

The **One-shot** checkbox in an Input node allows you to model this behavior:

- When **enabled**, the input node will only provide material during the **first recycling iteration** of each run.
- For all subsequent iterations in that run, the node is effectively **empty** — it doesn't inject additional material.





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# Run the Simulation

With your flowsheet built and variables configured, you're ready to execute the simulation.

In this section, you'll learn how to:

- Launch the simulation using the **Run** button
- Interpret **node status indicators** during execution



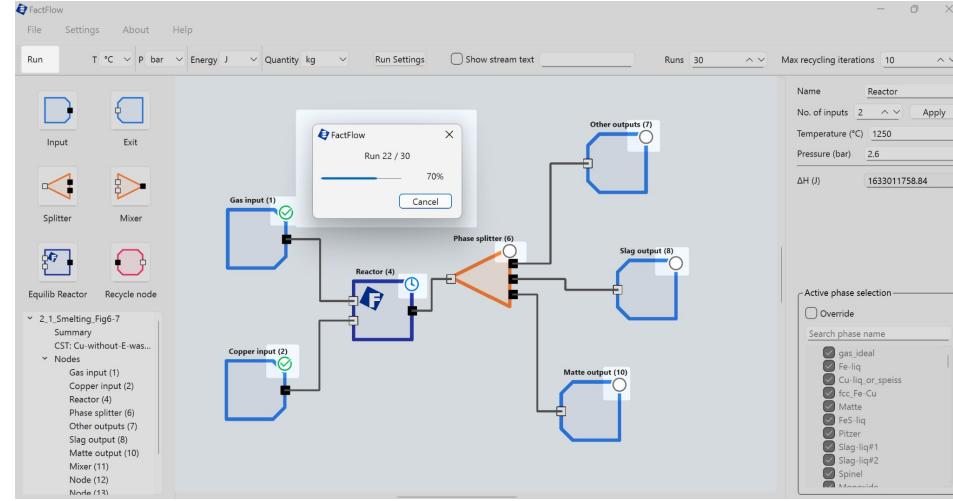
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# Run the Simulation



Once everything is set up, you can **launch your simulation** by clicking the **Run** button at the top left of the FactFlow window.

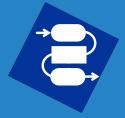
While the simulation is running, each node displays a **status icon** to show its current state:

**Idle** – The node is waiting to be calculated.

**Calculating** – The node is actively processing.

**Success** – The node completed its calculation without errors.

**Error** – The node encountered an issue.



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# Analyzing Results

Once your simulation has completed, it's time to explore and interpret the results.

In this section, you'll learn how to:

- View **stream results** directly from any node
- Use the **Analysis Module** to generate plots and compare results across runs

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# Analyzing Results

| Inputs                 |        |          | Outputs     |        |          |             |              |  |
|------------------------|--------|----------|-------------|--------|----------|-------------|--------------|--|
| Search name            |        |          | Search name |        |          |             |              |  |
| Name                   | Phase  | Quantity | Name        | Phase  | Quantity | Activity    | G            |  |
| CuFeS2_Chalcopyrite(s) | Solid  | 920      | > gas_ideal | Gas    | 620.221  |             |              |  |
| > gas_ideal            | Gas    | 434.483  | Matte       | Liquid | 575.504  |             |              |  |
| H2O_liquid(liq)        | Liquid | 80       | Cu          |        | 307.393  | 0.0467309   | -5.71227E+08 |  |
|                        |        |          | S           |        | 149.22   | 0.00658013  | -7.42042E+08 |  |
|                        |        |          | Fe          |        | 118.891  | 0.00771199  | -3.02666E+08 |  |
|                        |        |          | Slag-liq#1  | Liquid | 159.94   |             |              |  |
|                        |        |          | FeO         |        | 73.6488  | 0.444742    | -4.43326E+08 |  |
|                        |        |          | FeS         |        | 38.4982  | 0.245642    | -1.32088E+08 |  |
|                        |        |          | Fe2O3       |        | 22.3644  | 0.0326024   | -1.6179E+08  |  |
|                        |        |          | Fe2S3       |        | 12.4376  | 6.07677E-07 | -4.56314E+07 |  |
|                        |        |          | Cu2O        |        | 8.80621  | 6.00321E-05 | -3.24004E+07 |  |
|                        |        |          | Cu2S        |        | 4.18437  | 0.189183    | -1.04014E+07 |  |
|                        |        |          | SiO2        |        | 0        | 0           | 0            |  |
|                        |        |          | SiS2        |        | 0        | 0           | 0            |  |
|                        |        |          | > Spinel    | Solid  | 78.8178  |             |              |  |

Iteration 15 ▲▼

Export calculation log

After the simulation finishes, you can view the results from **any node** in the flowsheet.

- Double-click a node to open its **Results** window
- For **Exit** nodes, results are accessible via the Inspector

The **Results** window displays:

- The **phases and constituents** present at that point in the process
- Their corresponding **quantities, activities, and Gibbs energy (G)** (when applicable)

For **Equilib Reactor** nodes, you can also click **Export calculation log** to save a detailed record of the equilibrium calculation. This log is the same as what would be generated by **FactSage** for that iteration.



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# Analyzing Results - Plotting

|              |         |                         |              |      |
|--------------|---------|-------------------------|--------------|------|
| ▼ Slag-liq#1 | Liquid  | 159.94                  |              |      |
| FeO          | 73.6488 | 0.444742                | -4.43326E+08 | E+07 |
| FeS          | 38.4982 | 0.245642                | -1.32088E+08 | E+07 |
| Fe2O3        | 22.3644 | 0.0326024               | -1.6179E+08  | E+07 |
| Fe2S3        | 12.4376 | Plot analysis           |              |      |
| Cu2O         | 8.80621 | Plot elemental analysis |              |      |
| Cu2S         | 4.18437 | 0.189185                | -1.04014E+07 | E+07 |
| SiO2         | 0       | 0                       | 0            |      |
| Al2O3        | 0       | 0                       | 0            |      |

To create a plot, **right-click** any row in the Results window.

You'll see two options:

- **Plot analysis** – Plot quantities for the selected phases and species
- **Plot elemental analysis** – Plot total elemental amounts

## Selecting What to Plot

You can select one or more species using standard multi-selection methods:

- **Click and drag** to select a group
- **Shift-click** to select a range
- **Ctrl-click** to select or deselect individual rows

This allows you to customize exactly what gets sent to the **Analysis Module** for plotting.



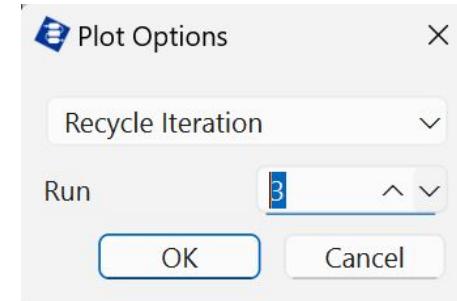
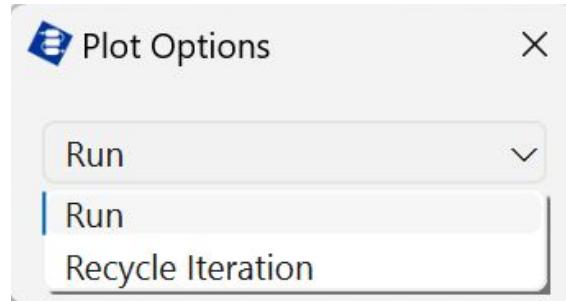
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# Analyzing Results - Plotting



Before generating your plot, the **Plot Options** dialog will appear.

This lets you choose what the x-axis of the plot should represent:

- **Run** – Plot how values change across parametric runs
- **Recycle Iteration** – Plot how values evolve within a single run, across recycling iterations

If you select **Recycle Iteration**, an additional field will appear allowing you to specify **which Run** to analyze. Each run has its own internal recycle history, so this selection determines which run's iterations will be plotted.

Click **OK** to proceed to the Analysis Module with your selected view.



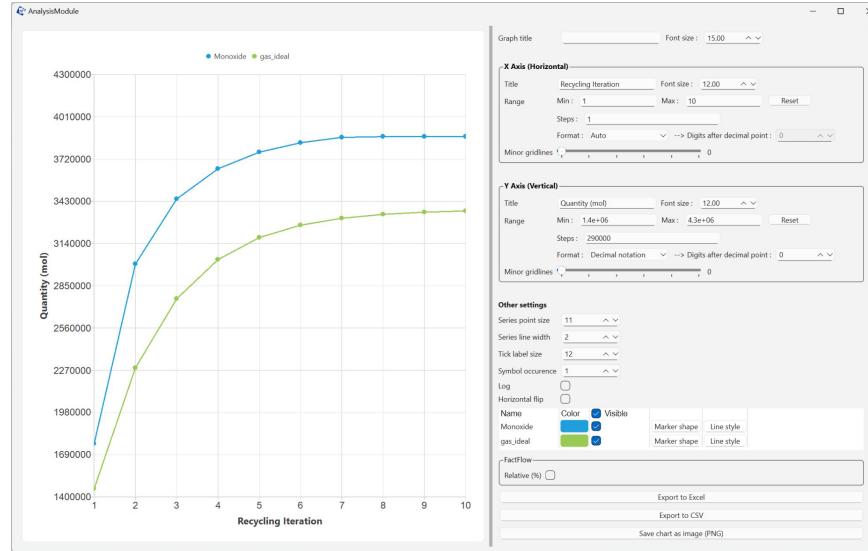
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# Analyzing Results - Plotting



The plot will open in the **Analysis Module** — a dedicated space for exploring and customizing your simulation results.

Here, you can:

- Visualize how selected values change across **runs** or **recycling iterations**
- Switch between **absolute values** and **relative percentages** (e.g., weight % within a phase)
- Enable log scale, adjust axes, labels, and visual styles
- **Export** the plot as an image or download the data as CSV or Excel



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# Advanced Section – Function Builder

You've made it!

By now, you've learned how to prepare your system, build a flowsheet, configure variables, and analyze results.

This next section introduces the **Function Builder** — a powerful tool that lets you define values using **custom formulas**, **mathematical functions**, and even simple **programming logic** like if-else, for, and while.

If you're ready to go beyond basic variable inputs, this tool gives you full control.



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# Function Builder - Custom formulas

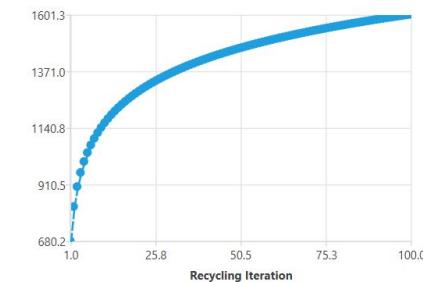
In any numeric input field, you can enter not just a number or variable name — but a **mathematical expression** using the Function Builder.

You can use:

- **Basic arithmetic:** +, -, \*, /, ^
- **Parentheses** for grouping: (A + B) / 2
- **Math functions:** sqrt(x), log(x), exp(x), abs(x), min(a, b), max(a, b)
- **Constants:** pi, e

You can also reference any **Run Variable** or **Recycle Iteration Variable** by name.

|                  |               |   |   |       |
|------------------|---------------|---|---|-------|
| No. of inputs    | 4             | ^ | ▼ | Apply |
| Temperature (°C) | 200*log(i*30) |   |   |       |
| Pressure (atm)   | 1             |   |   |       |



## Built-in variables

- **run** → the current run index (starting from 1)
- **i** → the current recycling iteration index (starting from 1)

Expressions are evaluated automatically for each run or iteration, allowing fully dynamic behavior.

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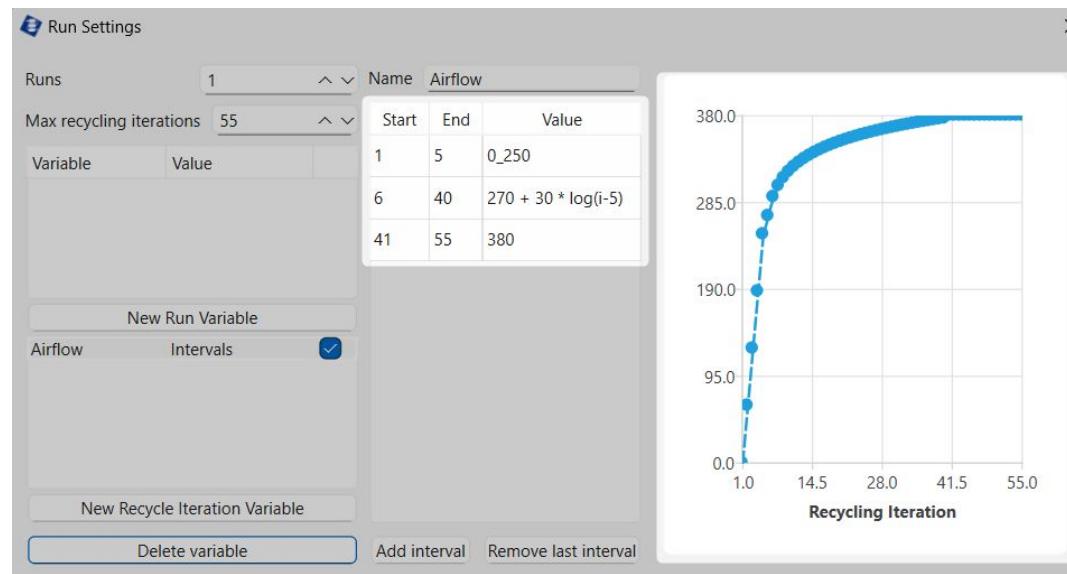


# Function Builder - Custom formulas

In addition to input fields, mathematical expressions can also be used in the **Value** column of the Run Settings panel — both in **basic** and **interval** modes.

This is especially powerful when using **Recycle Iteration Variables**, which can model **parameterized behaviour** as a function of the recycling iteration.

**Example:** Suppose you're simulating an oxidation step in a converter. Air flow can be increased with each iteration depending on user setting:



This allows you to model:

- **A diffusion-limited stage**
- **A steady-state plateau**

All within a single simulation run.



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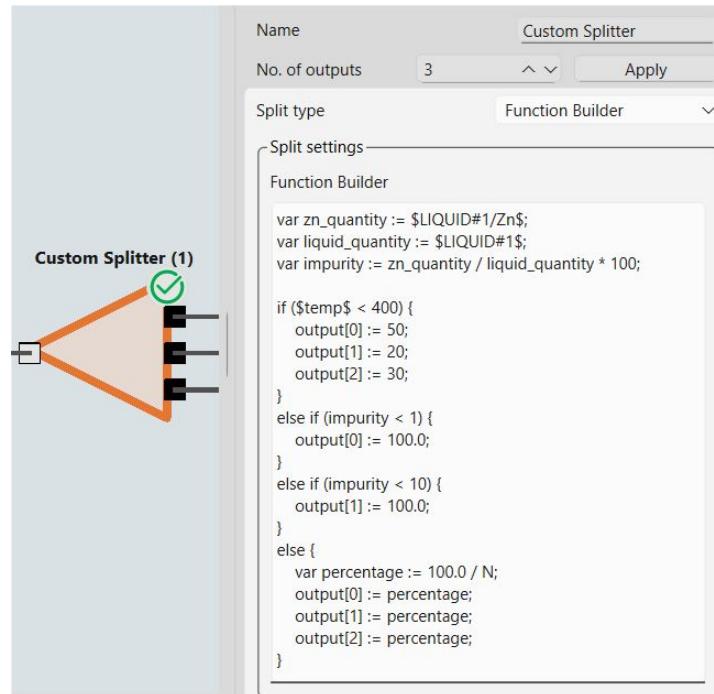
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# Function Builder - Splitter

In addition to using the Function Builder in input fields and variables, you can also use it directly in the **Splitter** node to control how material is routed between outputs. To enable this, set the **Split type** to **Function Builder** in the node's Inspector.

Instead of assigning fixed split percentages, the Function Builder lets you use **formulas** and **conditional logic** (if, else if, else) to dynamically control the split based on the input stream's composition or conditions.



In this example, the output is split differently depending on the **temperature** and the **Zn impurity** in a liquid phase.

## Built-in Variables for Splitters

- **\$Phase\$** or **\$Phase/Constituent\$** – quantity in the input stream
- **\$temp\$, \$pressure\$** – input stream conditions
- **output[index]** – array for assigning output split percentages
- **N** – total number of outputs



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# Support

We hope this guide has helped you get the most out of FactFlow and explore its full potential.

Should you run into any issues, have suggestions, or want to share feedback, we'd love to hear from you. Please don't hesitate to reach out at [factflow@polymtl.ca](mailto:factflow@polymtl.ca).

Our team is here to help and always looking for ways to improve your experience with FactFlow.