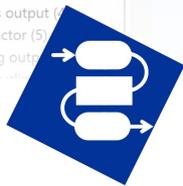
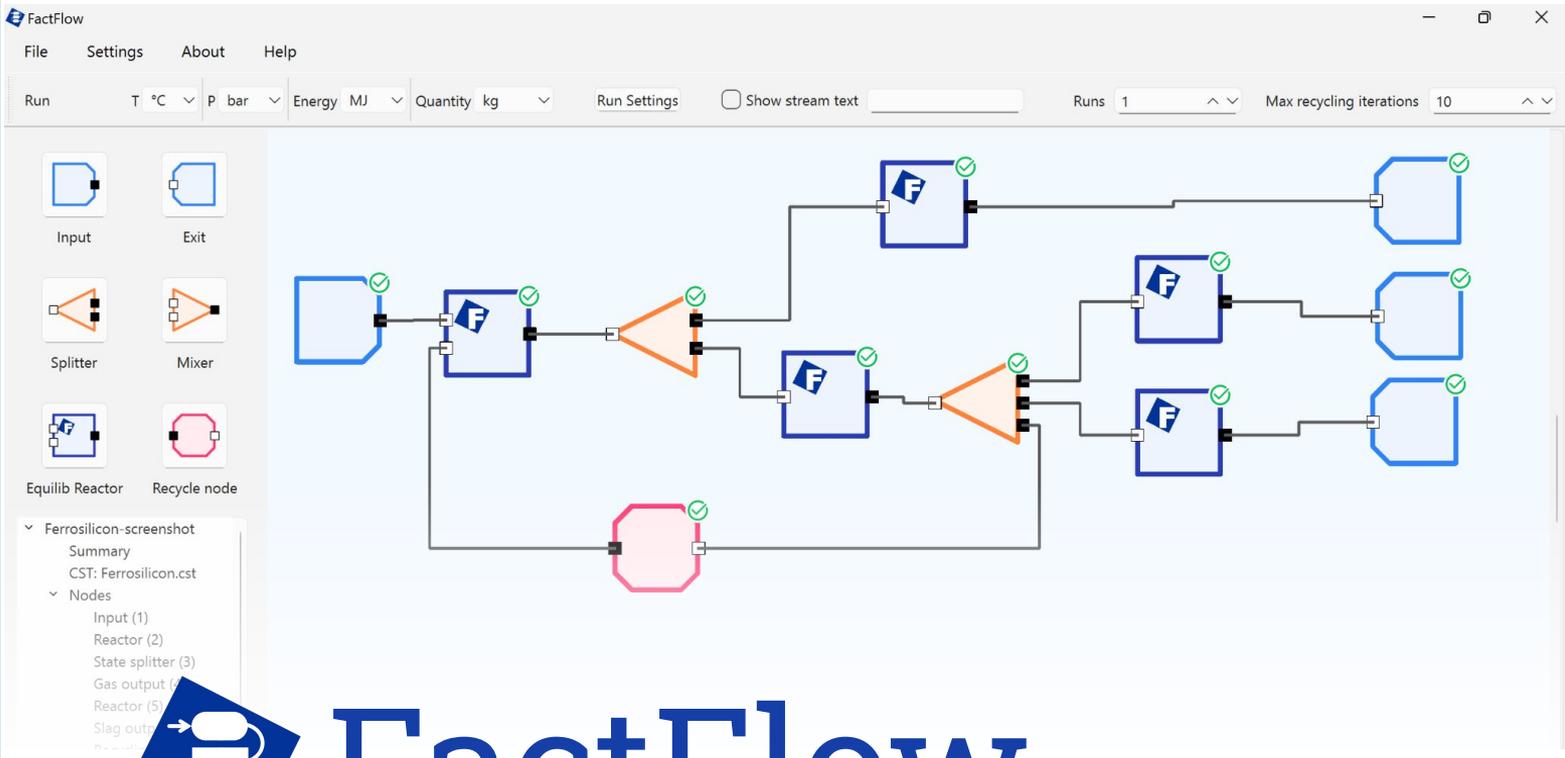


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FactFlow

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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.

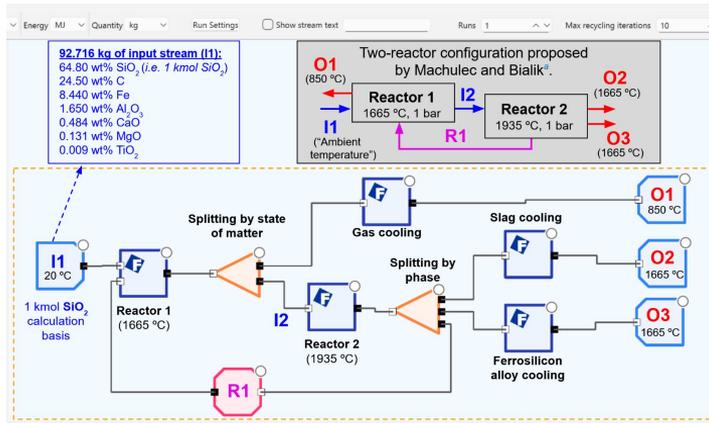
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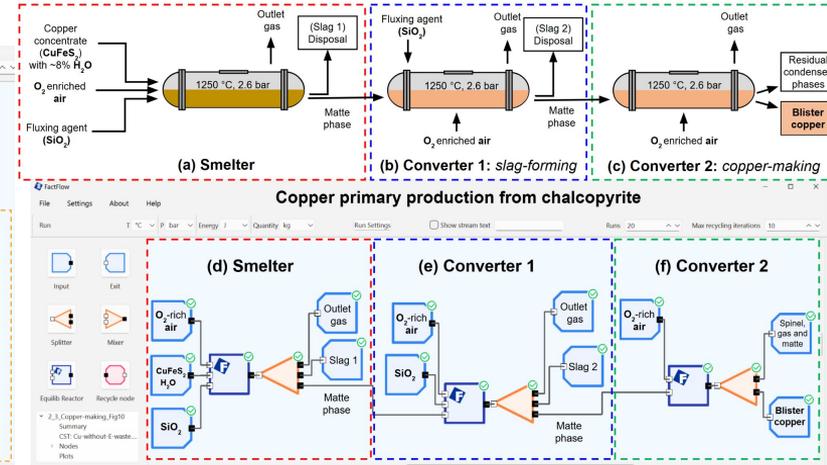
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FactFlow has already been employed to model various processes, and has been used by industry partners around the world.

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

<https://doi.org/10.1016/j.calphad.2024.102772>

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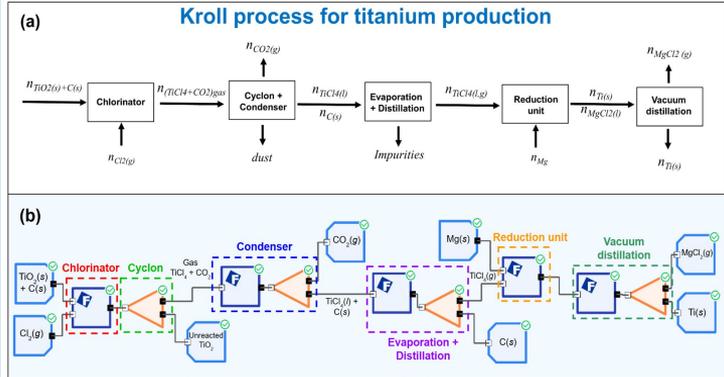
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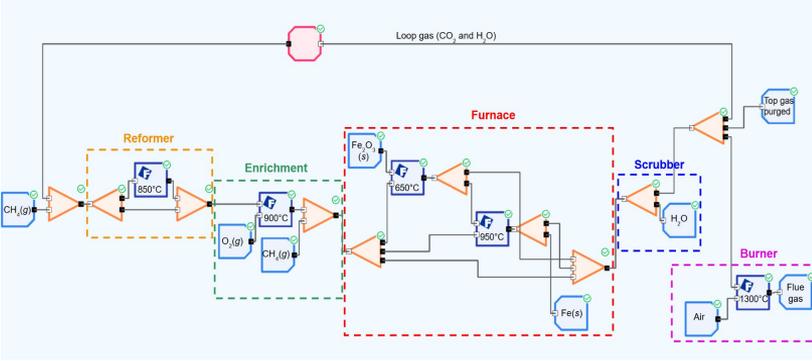
What is FactFlow?

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:



Titanium primary production



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.

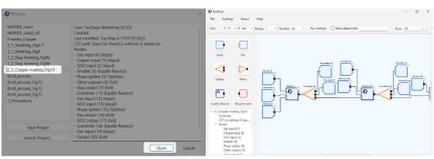
We strongly recommend beginning with the **Getting Started** section. It's a guided walkthrough that shows you how to **reproduce a real figure** from the FactFlow paper, step by step.

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.

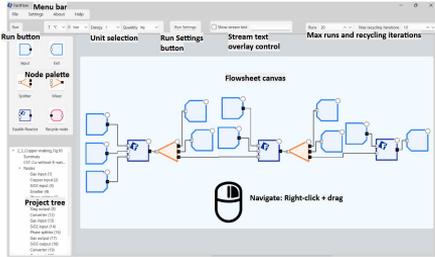
Getting Started - Open an example



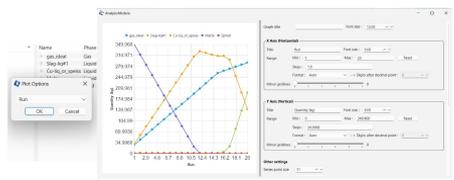
FactFlow examples are a great way to learn how the software works and explore its capabilities. To open an example, select it from the list and click **Open** in the bottom-right corner.

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



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.

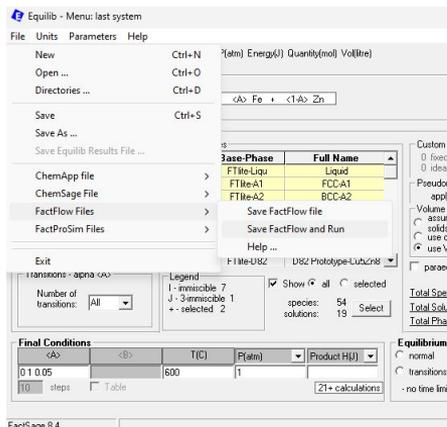
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What Comes Next - Creating your own Process Simulation

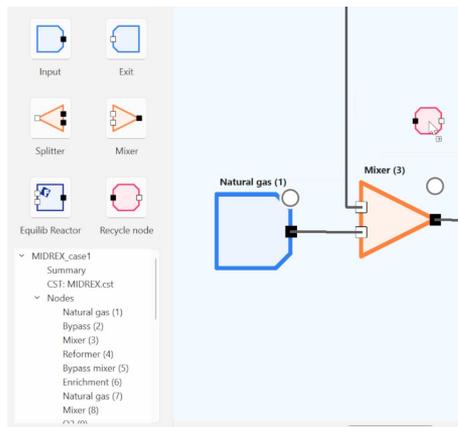
To create your own simulation, you'll follow a multi-step process. Each of these steps is explained in detail in this manual.



Step 1

Prepare your Database

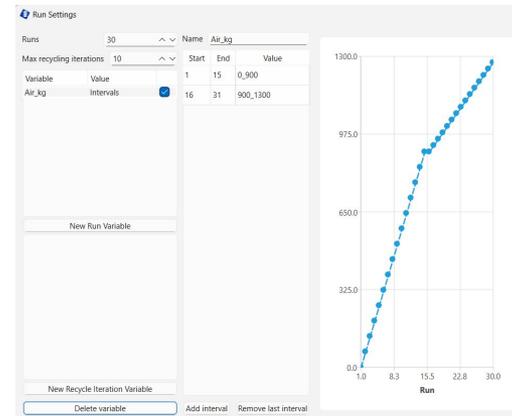
Use FactSage's Equilib module to perform the species and phase selection for your flowsheet's mini database.



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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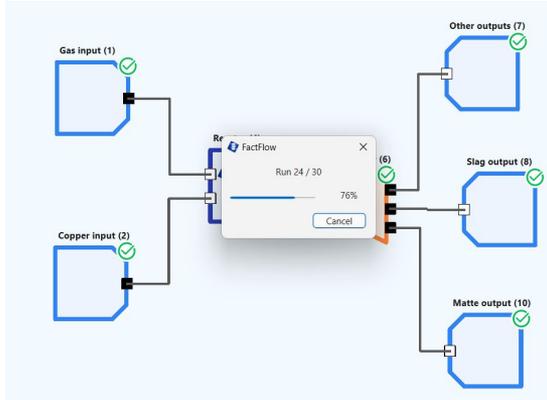
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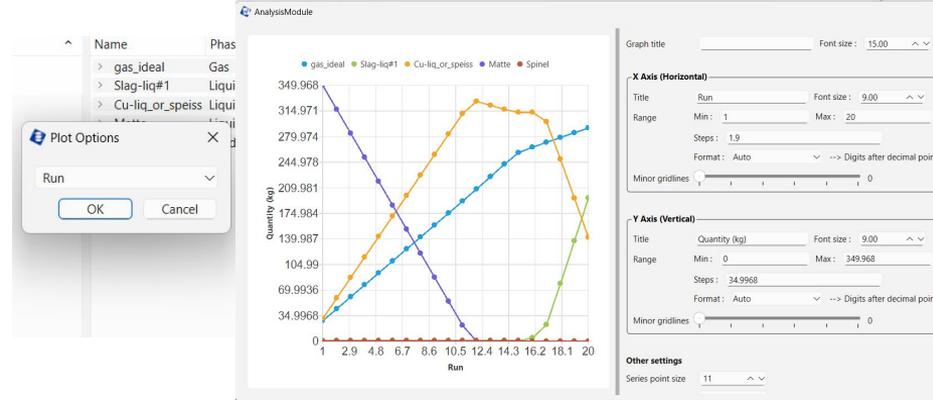
What Comes Next - Creating your own Process Simulation

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

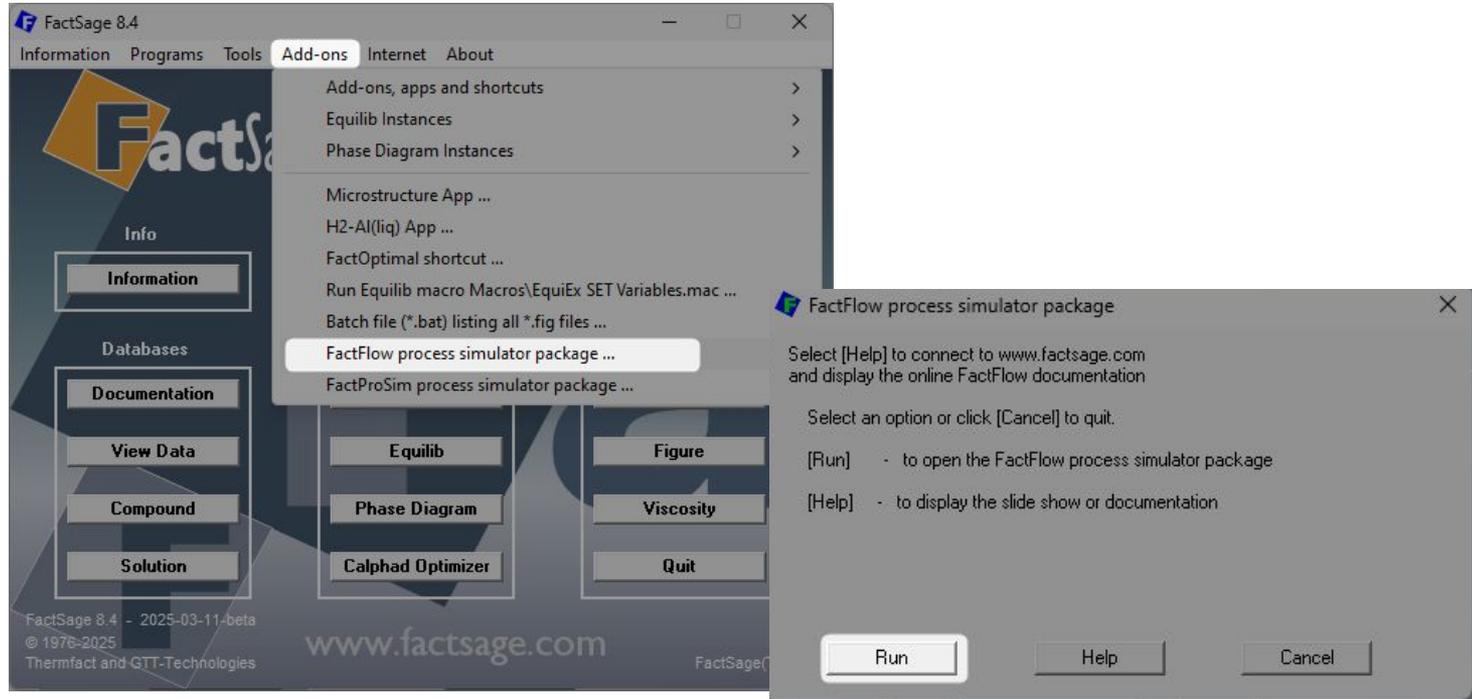
Before launching FactFlow, make sure your system meets the following requirements:



- **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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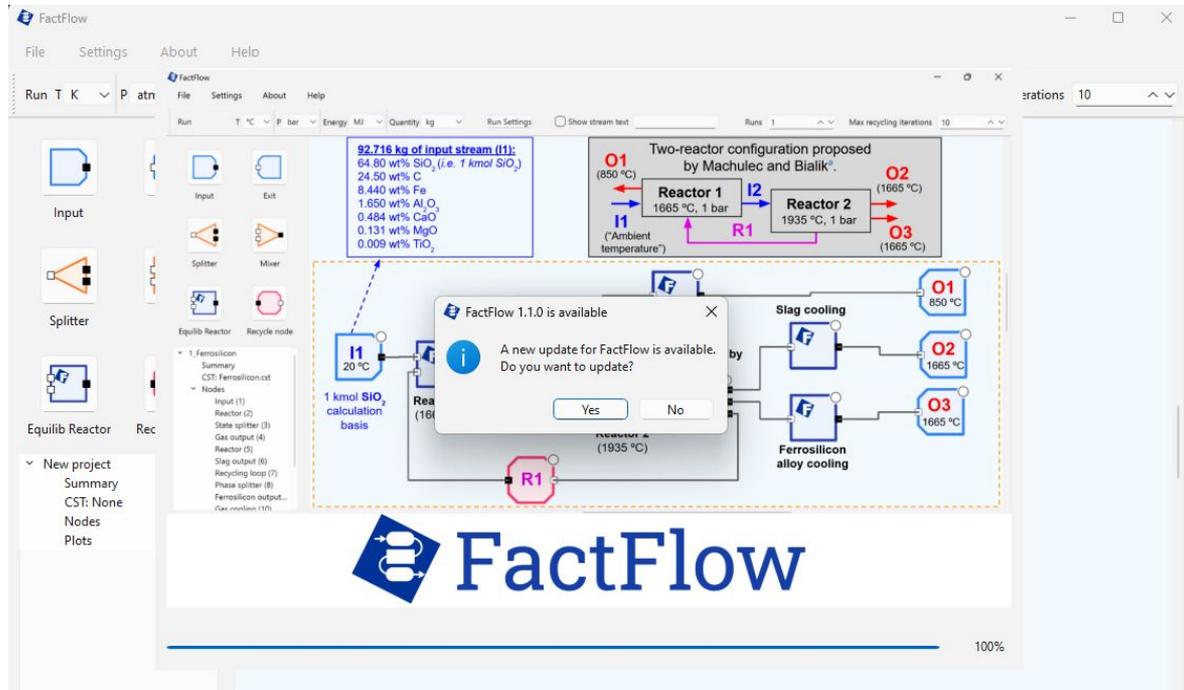


To launch FactFlow, open **FactSage**, then go to the **Add-ons** menu in the top toolbar and select **FactFlow process simulator package...** from the dropdown list. Click **Run** to launch FactFlow in the pop-up window.

Getting Started - Launching FactFlow

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The screenshot displays the FactFlow software interface. The main window shows a simulation setup for a two-reactor configuration. The input stream (I1) is defined as 92.716 kg of input stream (I1) with the following composition: 64.80 wt% SiO₂ (i.e. 1 kmol SiO₂), 24.50 wt% C, 8.440 wt% Fe, 1.650 wt% Al₂O₃, 0.484 wt% CaO, 0.131 wt% MgO, and 0.009 wt% TiO₂. The simulation parameters are set to Run T, K, P, bar, Energy, MJ, Quantity, kg, with Run Settings showing 10 Max recycling iterations. The reactor configuration includes Reactor 1 (1665 °C, 1 bar) and Reactor 2 (1935 °C, 1 bar). The output streams are O1 (850 °C), O2 (1665 °C), and O3 (1665 °C). A dialog box is open in the center, titled "FactFlow 1.1.0 is available", with the message "A new update for FactFlow is available. Do you want to update?" and "Yes" and "No" buttons.

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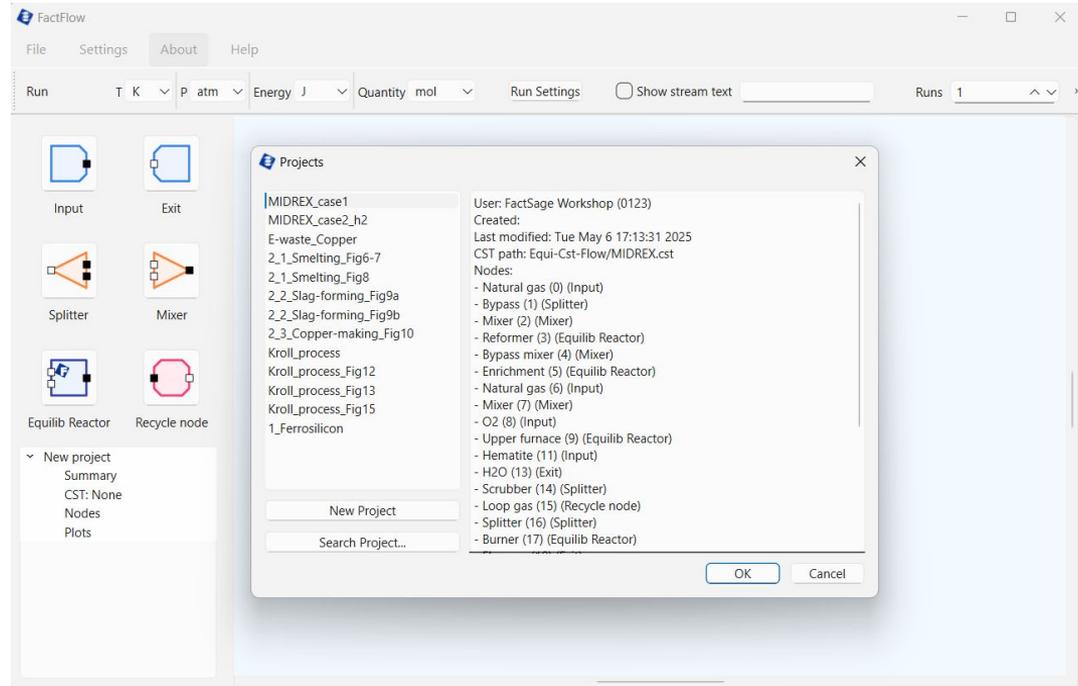


On launch, FactFlow may prompt you to install an available update. We **highly recommend** clicking **Yes**—the update will run automatically, and FactFlow will relaunch once it's complete.

Getting Started - Projects window

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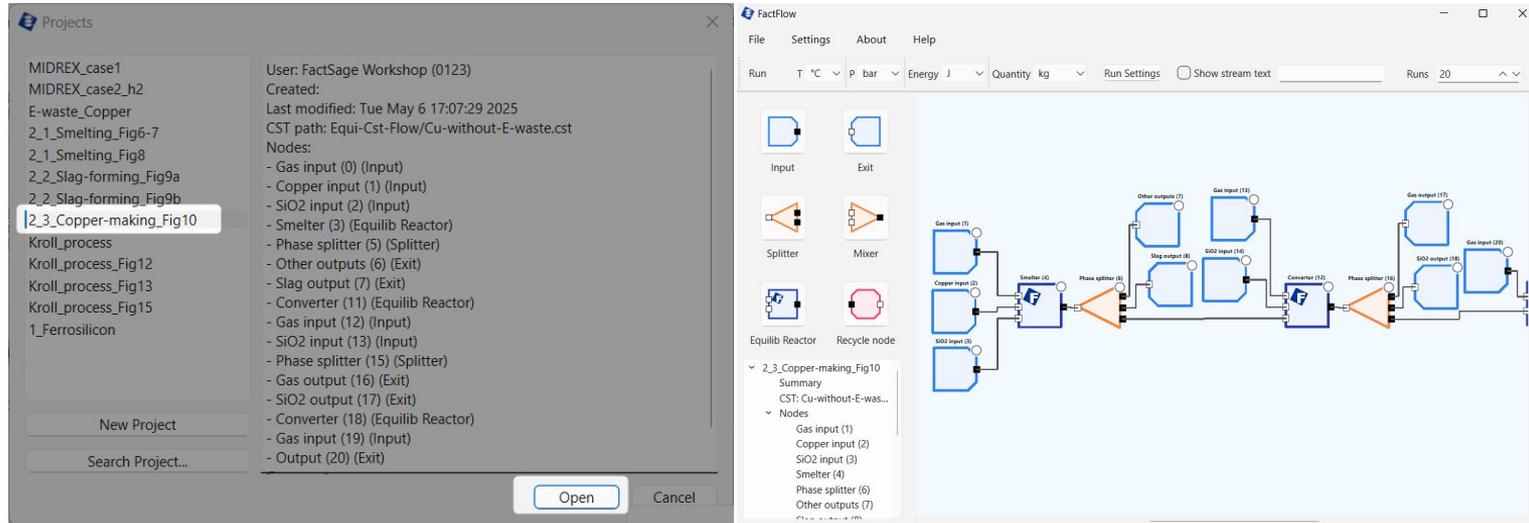
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Upon launch, FactFlow automatically opens the **Projects** window, where you can view, open, or create projects.

Getting Started - Open an example

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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.

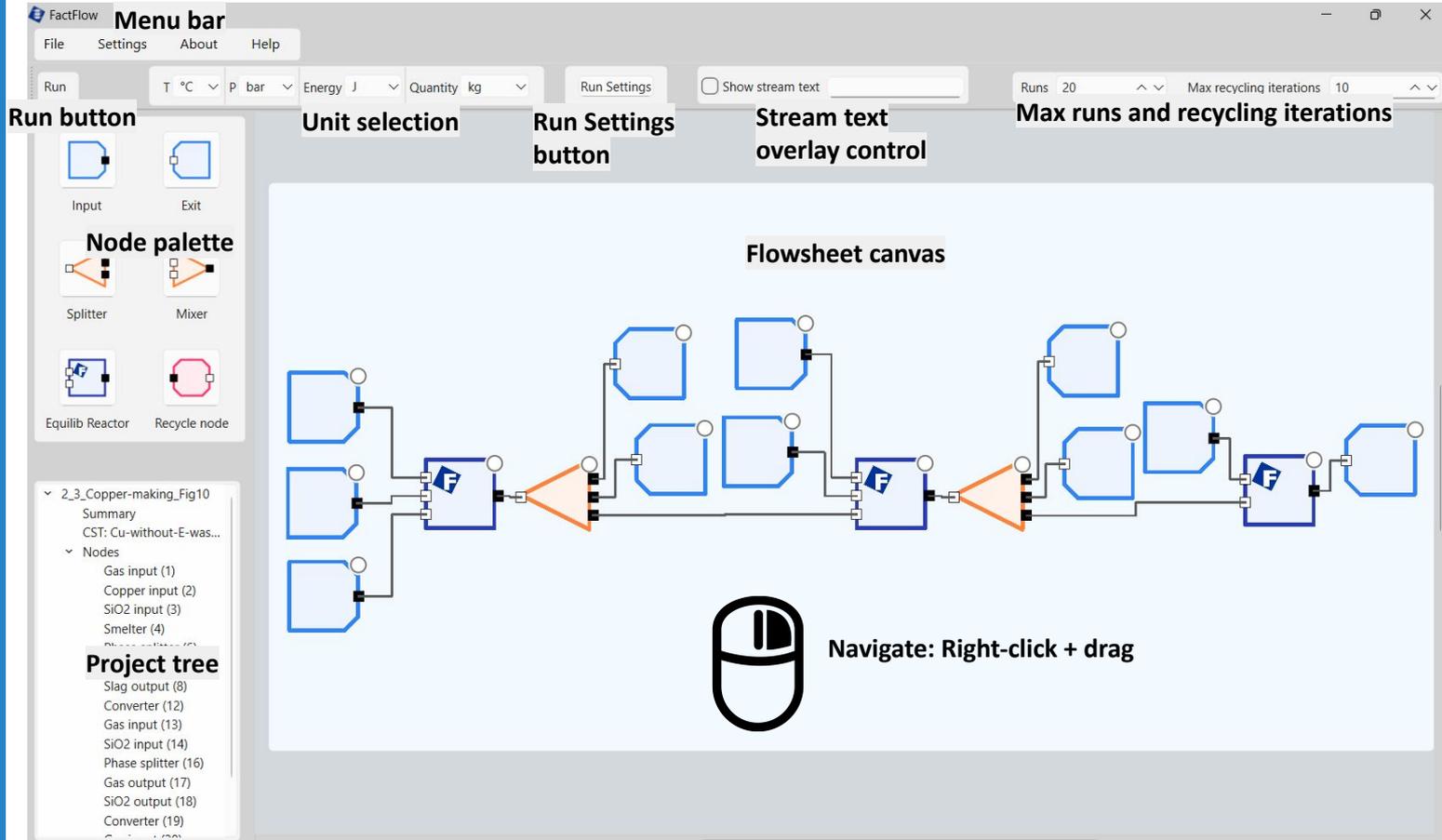
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Getting Started - Main interface

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The screenshot displays the FactFlow software interface. At the top is a **Menu bar** with options: File, Settings, About, Help. Below the menu bar are several control elements: a **Run button**, **Unit selection** (Temperature: T °C, Pressure: P bar, Energy: Energy J, Quantity: kg), **Run Settings** (Run Settings button), **Stream text overlay control** (Show stream text checkbox), and **Max runs and recycling iterations** (Runs: 20, Max recycling iterations: 10).

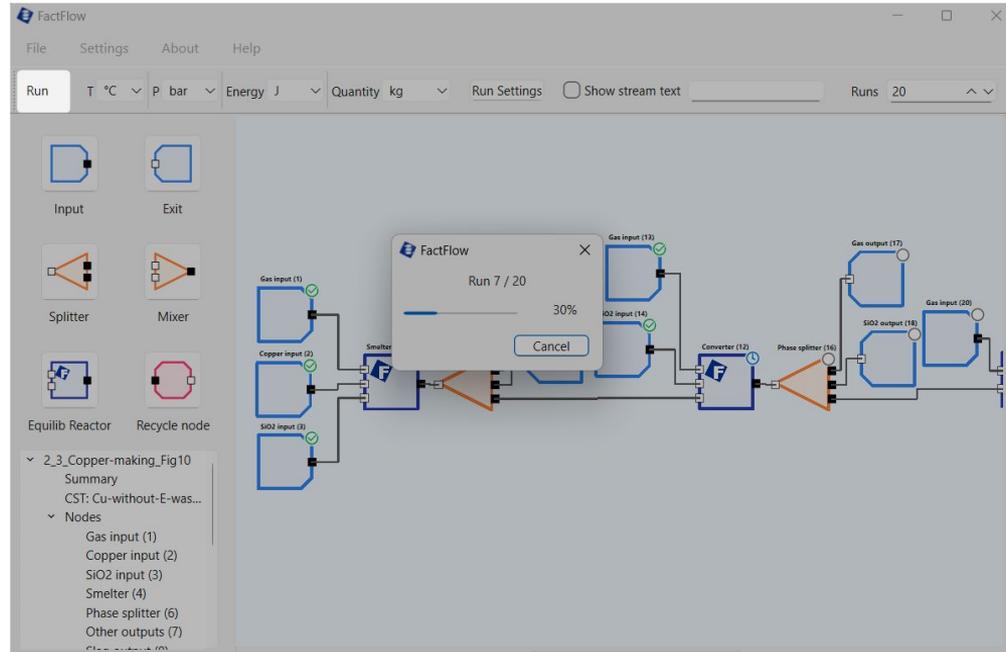
The main area is the **Flowsheet canvas**, which contains a complex process flow diagram. On the left side, there is a **Node palette** with icons for Input, Exit, Splitter, Mixer, Equilib Reactor, and Recycle node. At the bottom left, there is a **Project tree** showing a hierarchy for a project named '2_3_Copper-making_Fig10', including a Summary and a list of Nodes such as Gas input (1), Copper input (2), SiO2 input (3), Smelter (4), Slag output (8), Converter (12), Gas input (13), SiO2 input (14), Phase splitter (16), Gas output (17), SiO2 output (18), and Converter (19).

At the bottom center, there is a mouse icon with the text **Navigate: Right-click + drag**.

Getting Started - Run a calculation

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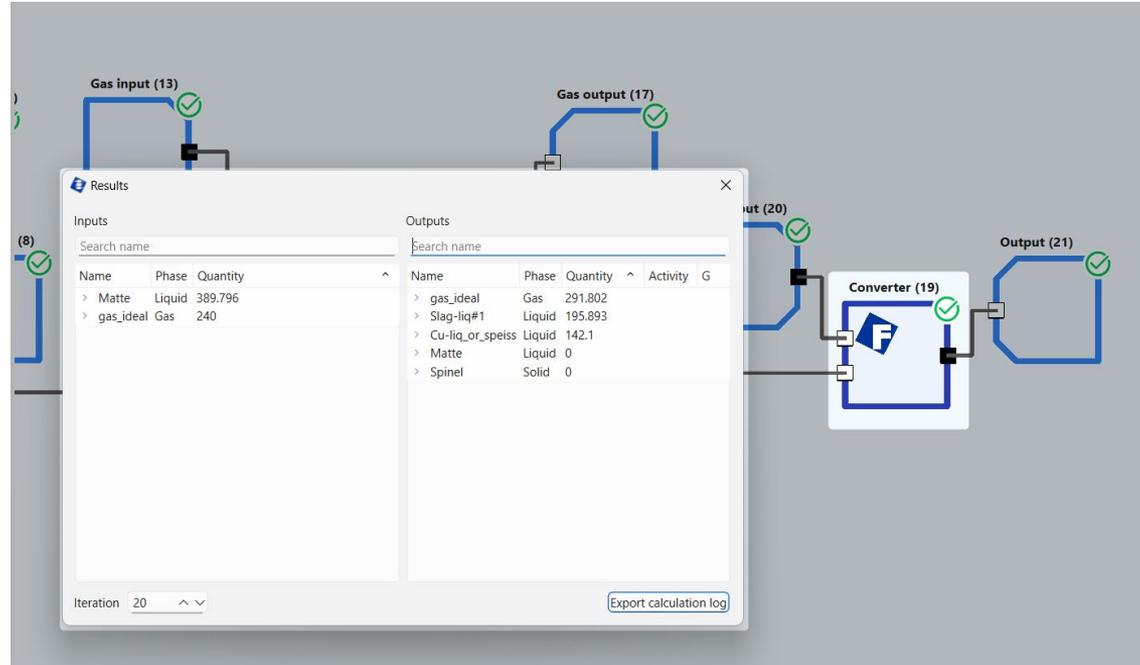
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Let's run the example. Click the **Run** button at the top left and wait for the simulation to complete. This example is set up to perform **20 runs, varying the amount of O₂-enriched air input** in the second converter. You'll learn how to build your own flowsheet and configure runs later in the guide.

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The screenshot shows a simulation interface with a flowsheet. A 'Results' window is open, displaying the following data:

Inputs			Outputs				
Name	Phase	Quantity	Name	Phase	Quantity	Activity	G
> Matte	Liquid	389.796	> gas_ideal	Gas	291.802		
> gas_ideal	Gas	240	> Slag-liq#1	Liquid	195.893		
			> Cu-liq_or_speiss	Liquid	142.1		
			> Matte	Liquid	0		
			> Spinel	Solid	0		

At the bottom of the Results window, it shows 'Iteration: 20' and an 'Export calculation log' button.

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.

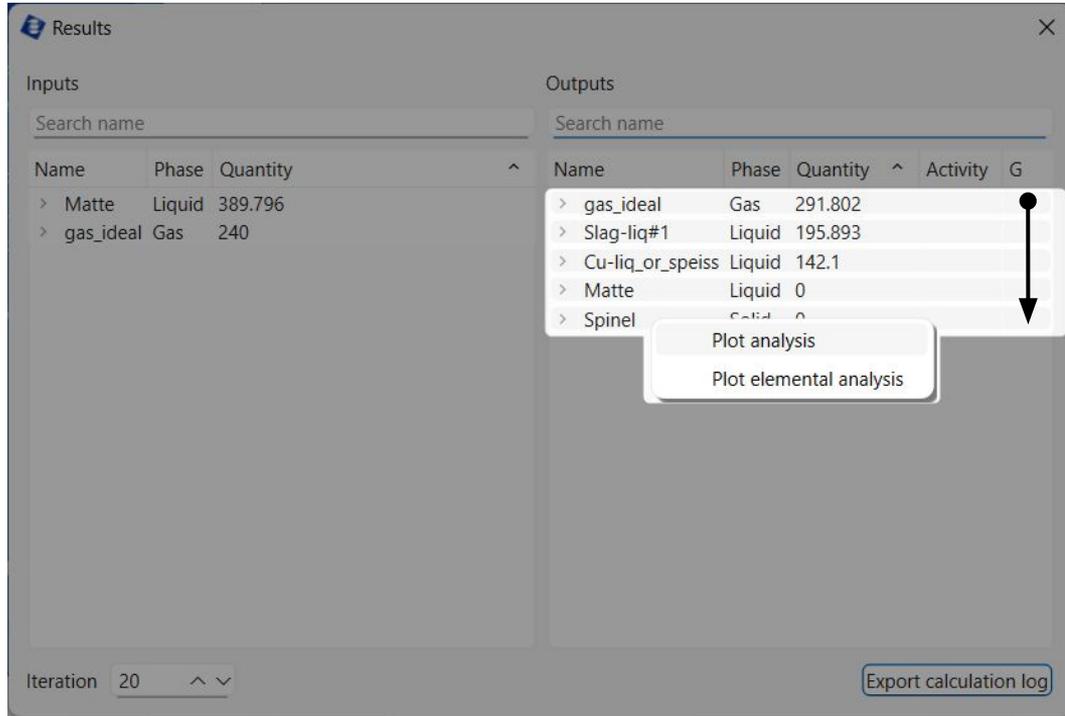
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The screenshot shows the 'Results' window with two panels: 'Inputs' and 'Outputs'. The 'Outputs' panel contains a table with columns: Name, Phase, Quantity, Activity, and G. A multi-select operation is shown where the first three rows are highlighted, and a context menu is open over the third row, offering 'Plot analysis' and 'Plot elemental analysis'. A mouse cursor is positioned over the 'Plot analysis' option. A vertical double-headed arrow indicates the range of selected rows.

Name	Phase	Quantity	Activity	G
> gas_ideal	Gas	291.802		
> Slag-liq#1	Liquid	195.893		
> Cu-liq_or_speiss	Liquid	142.1		
> Matte	Liquid	0		
> Spinel	Solid	0		

Iteration: 20 Export calculation log



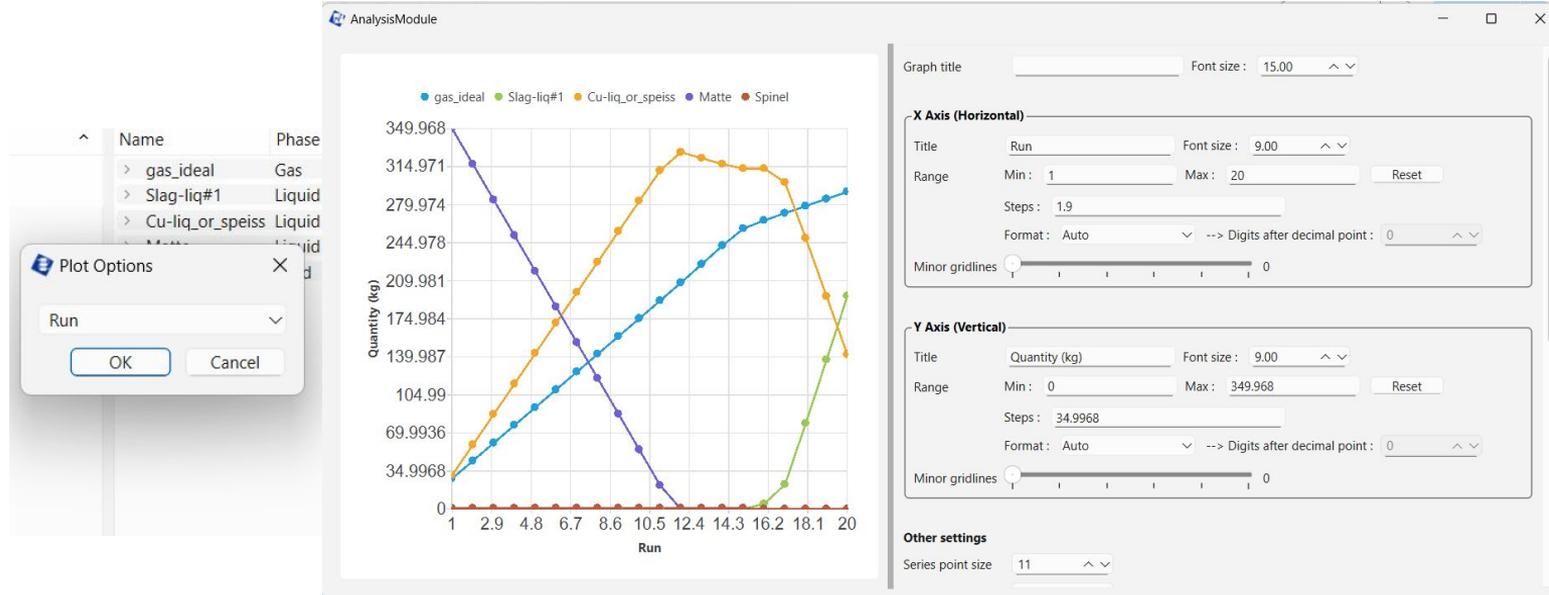
Multi-select: Left-click + drag

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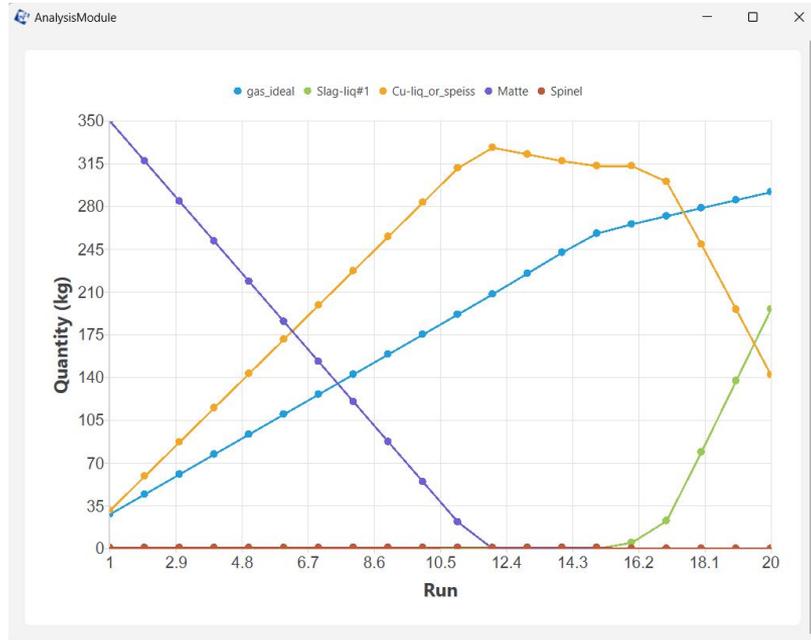
In the **Plot Options** dialog, simply **click OK**. This will launch the **Analysis Module**, FactFlow's dedicated environment for advanced analysis and visualization. Plot settings and customization options will be covered later in this guide.

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K. Poëti et al.

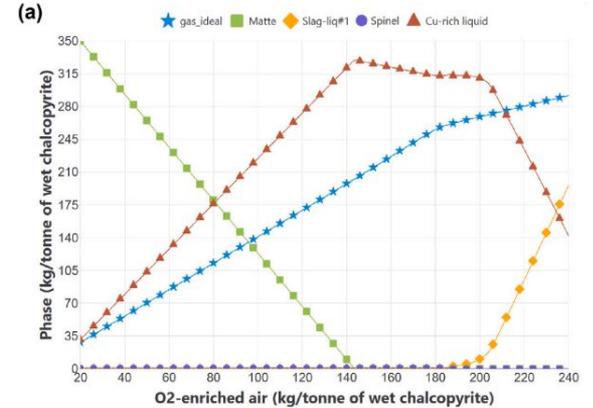


Fig. 10. (a) Phase assemblage evolution during the copper-making step (converter 2) as a function of the air injection in converter 2.

🎉 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.

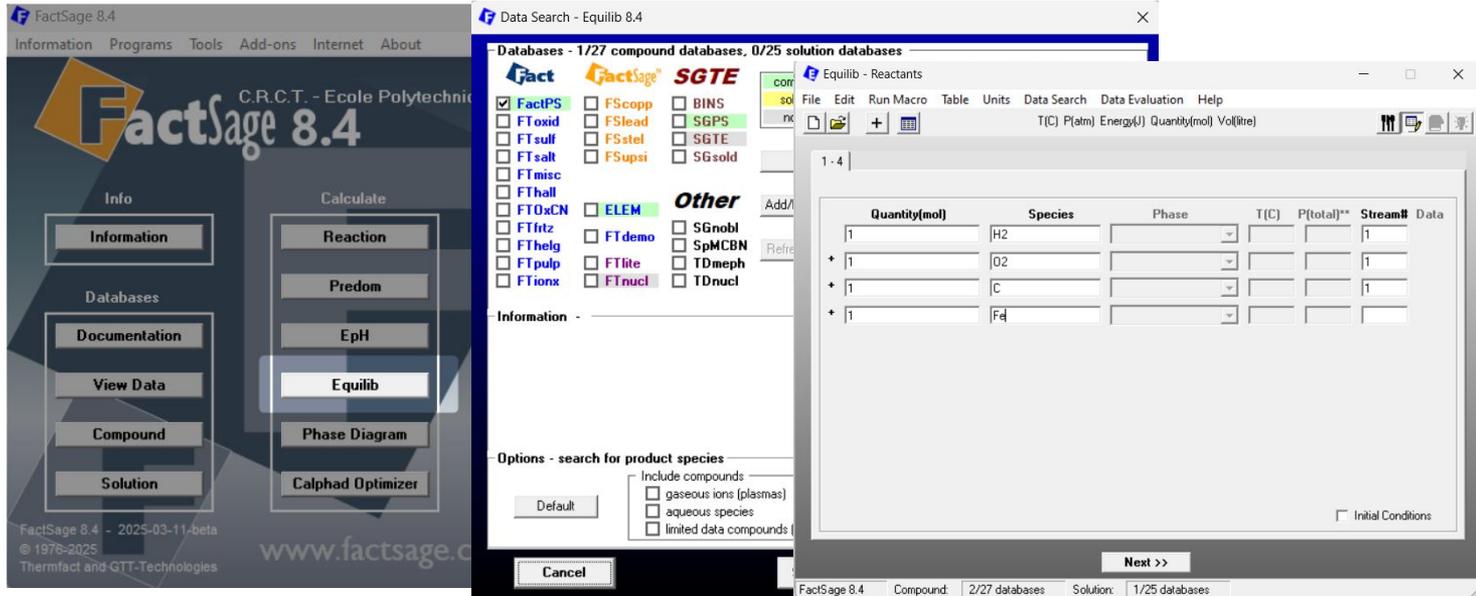
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The image shows two overlapping windows from the FactSage 8.4 software. The background window is the main application interface with the 'Equilib' module selected in the 'Calculate' column. The foreground window is the 'Data Search - Equilib 8.4' dialog box, which is used to select databases and input species for the equilibrium calculation.

Data Search - Equilib 8.4

Databases - 1/27 compound databases, 0/25 solution databases

Fact	FactSage	SGTE
<input checked="" type="checkbox"/> FactPS	<input type="checkbox"/> FScoep	<input type="checkbox"/> BINS
<input type="checkbox"/> FToxid	<input type="checkbox"/> FSlead	<input type="checkbox"/> SGPS
<input type="checkbox"/> FTsulf	<input type="checkbox"/> FSstel	<input type="checkbox"/> SGTE
<input type="checkbox"/> FTsalt	<input type="checkbox"/> FSupsi	<input type="checkbox"/> SGsold
<input type="checkbox"/> FTmisc		
<input type="checkbox"/> FTHall	<input type="checkbox"/> ELEM	Other
<input type="checkbox"/> FTxOxN	<input type="checkbox"/> FTdemo	<input type="checkbox"/> SGnobl
<input type="checkbox"/> FTfritz	<input type="checkbox"/> FTlite	<input type="checkbox"/> SpMCBN
<input type="checkbox"/> FThelp	<input type="checkbox"/> FTnucl	<input type="checkbox"/> TDmeph
<input type="checkbox"/> FTpulp		<input type="checkbox"/> TDnucl
<input type="checkbox"/> FTionx		

Options - search for product species

Include species

- gaseous ions (plasmas)
- aqueous species
- limited data compounds

Initial Conditions

Next >>

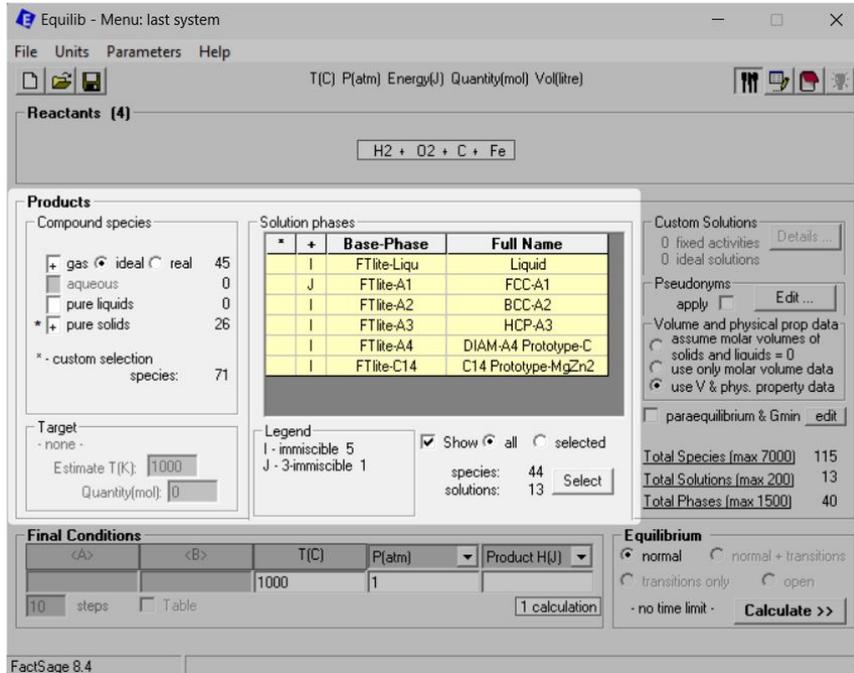
1. Launch the **Equilib** module in FactSage.
2. **Select the appropriate databases** in the Data Search menu.
3. **Enter the input species involved in your system.** The quantities can be arbitrary — they do NOT affect the mini-database used by FactFlow.

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Prepare your Database

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The screenshot shows the 'Equilib' software window with the following details:

- Reactants (4):** H₂ + O₂ + C + Fe
- Products:**
 - Compound species: gas (45), aqueous (0), pure liquids (0), pure solids (26), custom selection (71).
 - Target: none, Estimate T(K): 1000, Quantity(mol): 0.
- Solution phases table:**

*	+	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.
- Final Conditions:** T(C) = 1000, P(atm) = 1, Product H(J) = 1 calculation.
- Equilibrium:** normal selected, no time limit, **Calculate >>**
- Summary:** Total Species (max 7000) = 115, Total Solutions (max 200) = 13, Total Phases (max 1500) = 40.

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

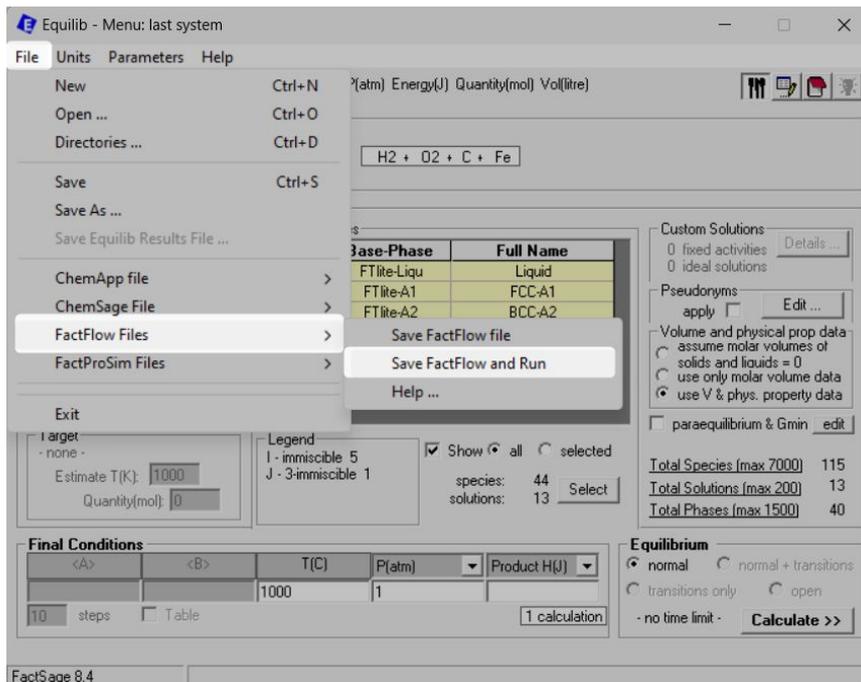
Temperature, pressure, and other calculation conditions do not affect the database generation and can be left unchanged.

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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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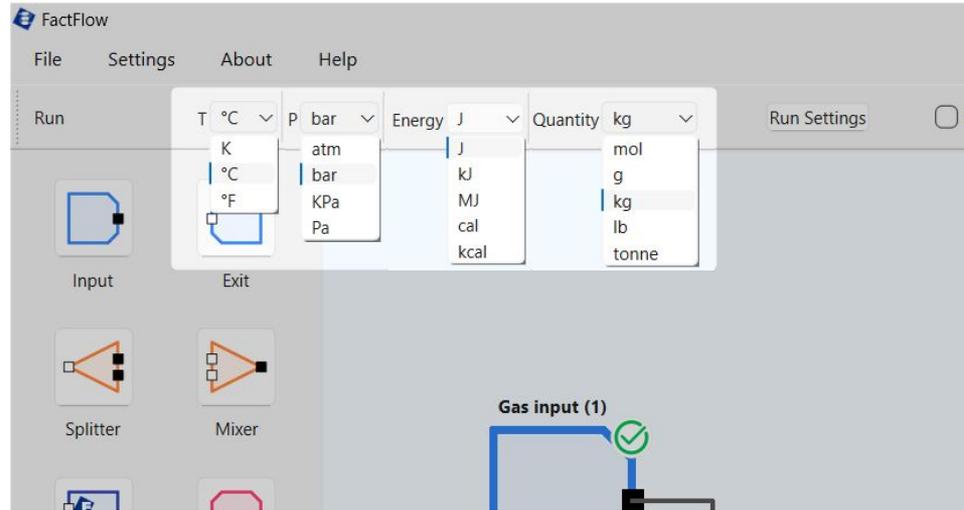
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Build the Flowsheet - Units selection



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**.

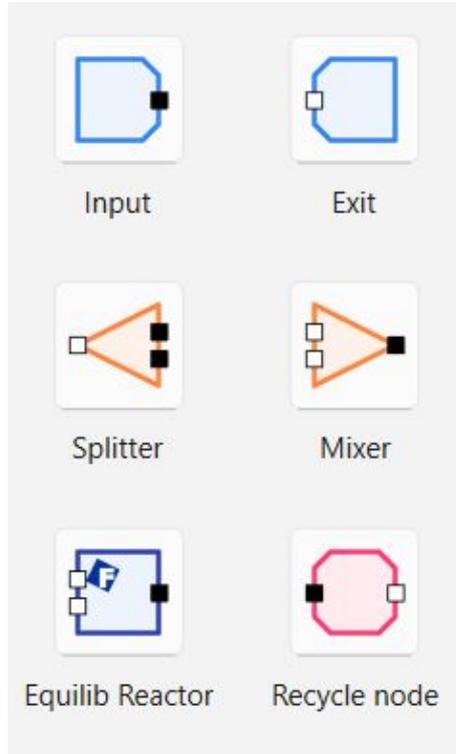
You can change these units at any time — they only affect how values are displayed and entered in the interface.

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Build the Flowsheet - Node Types

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



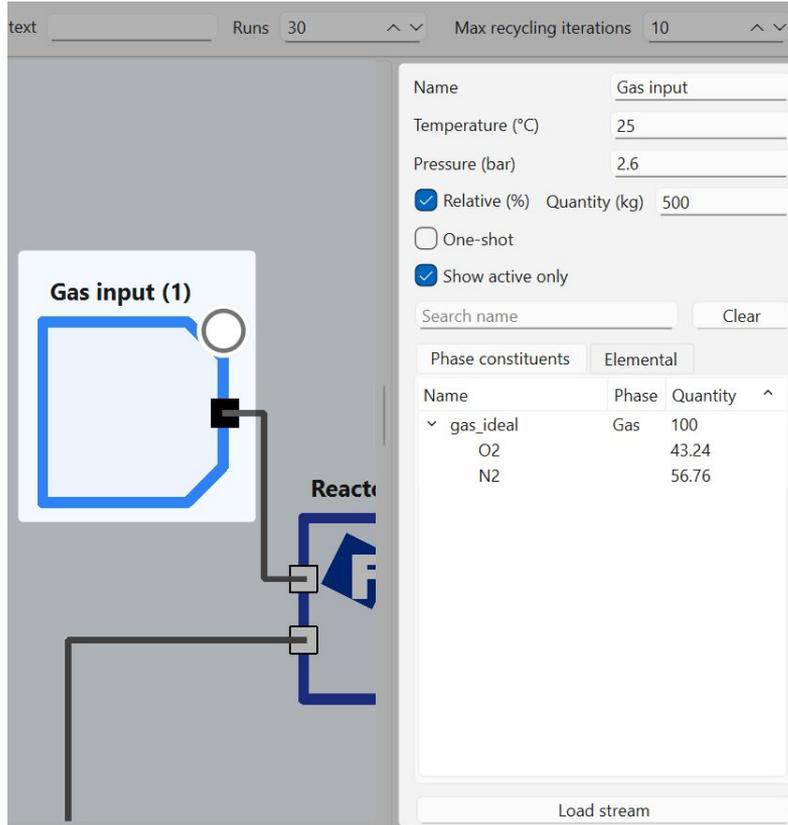
- **Input:** Defines an input stream, including phase or constituent quantities, as well as its temperature and pressure.
- **Exit:** Retrieves and displays the results of a given output stream for analysis.
- **Equilib Reactor:** Performs an equilibrium calculation using the same algorithm as FactSage.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

Build the Flowsheet - Input node

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



text Runs 30 Max recycling iterations 10

Gas input (1)

Reactor

Name: Gas input

Temperature (°C): 25

Pressure (bar): 2.6

Relative (%) Quantity (kg): 500

One-shot

Show active only

Search name: Clear

Phase constituents		Elemental
Name	Phase	Quantity
gas_ideal	Gas	100
O2		43.24
N2		56.76

Load stream

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)

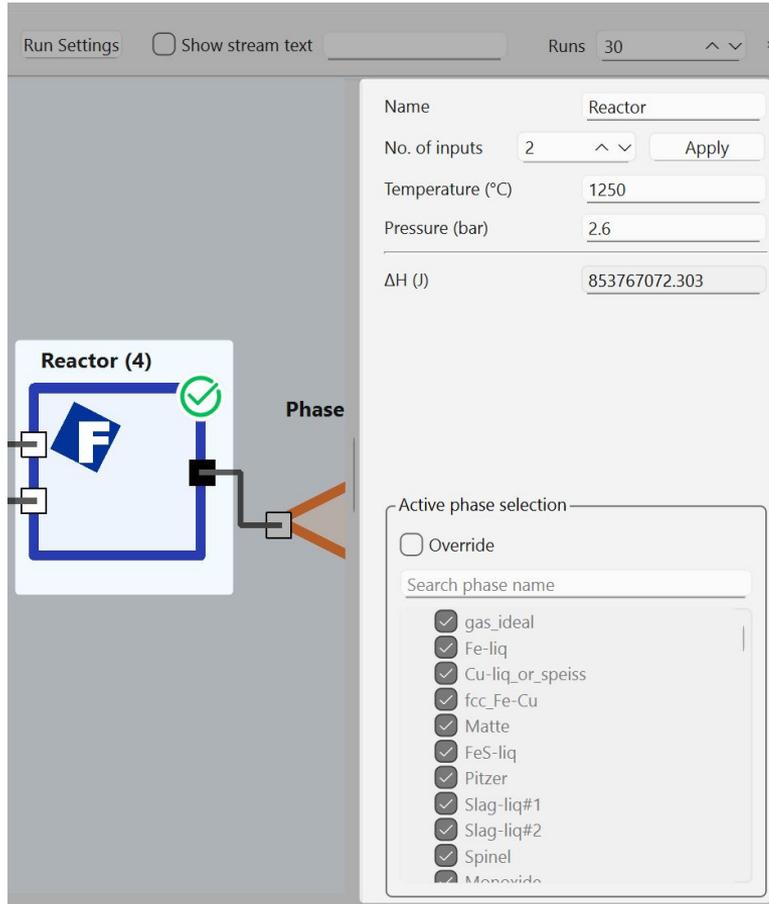
- Enter percentage values in the Quantity column
- Total must equal 100

Phase constituents		Elemental	
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



Run Settings Show stream text Runs 30

Name: Reactor

No. of inputs: 2

Temperature (°C): 1250

Pressure (bar): 2.6

ΔH (J): 853767072.303

Active phase selection

Override

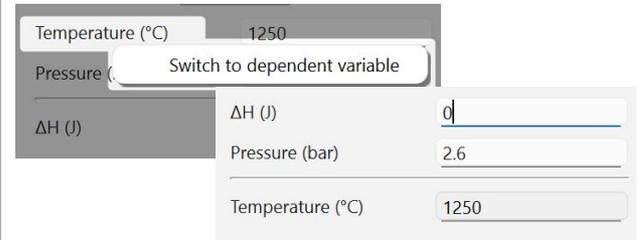
Search phase name

- gas_ideal
- Fe-liq
- Cu-liq_or_speiss
- fcc_Fe-Cu
- Matte
- FeS-liq
- Pitzer
- Slag-liq#1
- Slag-liq#2
- Spinel
- Monoxide

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.”



Temperature (°C) 1250

Pressure (bar) 2.6

ΔH (J) 853767072.303

Switch to dependent variable

ΔH (J) 0

Pressure (bar) 2.6

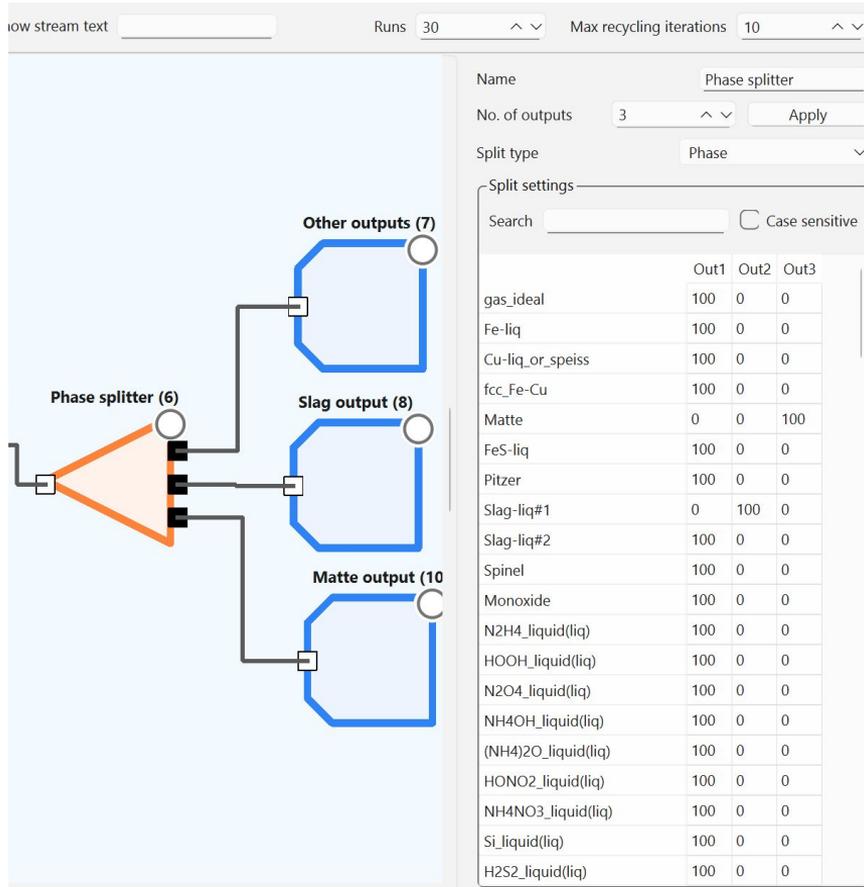
Temperature (°C) 1250

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

Build the Flowsheet - Splitter node

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low stream text Runs 30 Max recycling iterations 10

Name Phase splitter

No. of outputs 3 Apply

Split type Phase

Split settings

Search Case sensitive

	Out1	Out2	Out3
gas_ideal	100	0	0
Fe-liq	100	0	0
Cu-liq_or_speiss	100	0	0
fcc_Fe-Cu	100	0	0
Matte	0	0	100
FeS-liq	100	0	0
Pitzer	100	0	0
Slag-liq#1	0	100	0
Slag-liq#2	100	0	0
Spinel	100	0	0
Monoxide	100	0	0
N2H4_liquid(liq)	100	0	0
HOOH_liquid(liq)	100	0	0
N2O4_liquid(liq)	100	0	0
NH4OH_liquid(liq)	100	0	0
(NH4)2O_liquid(liq)	100	0	0
HONO2_liquid(liq)	100	0	0
NH4NO3_liquid(liq)	100	0	0
Si_liquid(liq)	100	0	0
H2S2_liquid(liq)	100	0	0

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.

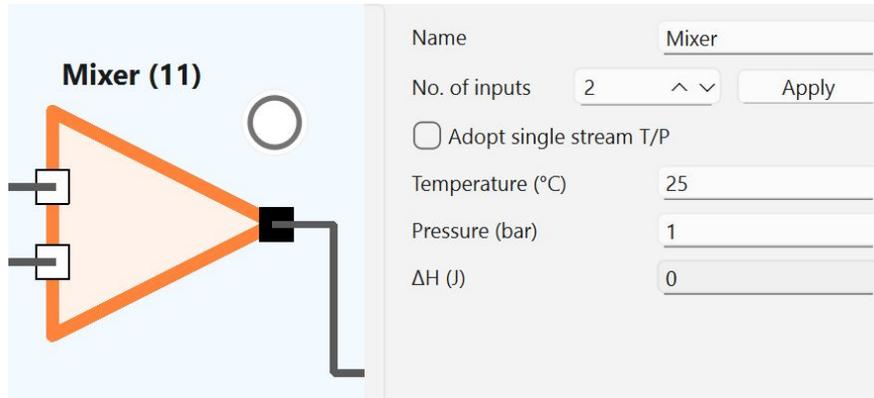
Use Splitter nodes when directing specific parts of a stream to different process paths.

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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.

Build the Flowsheet - Exit node

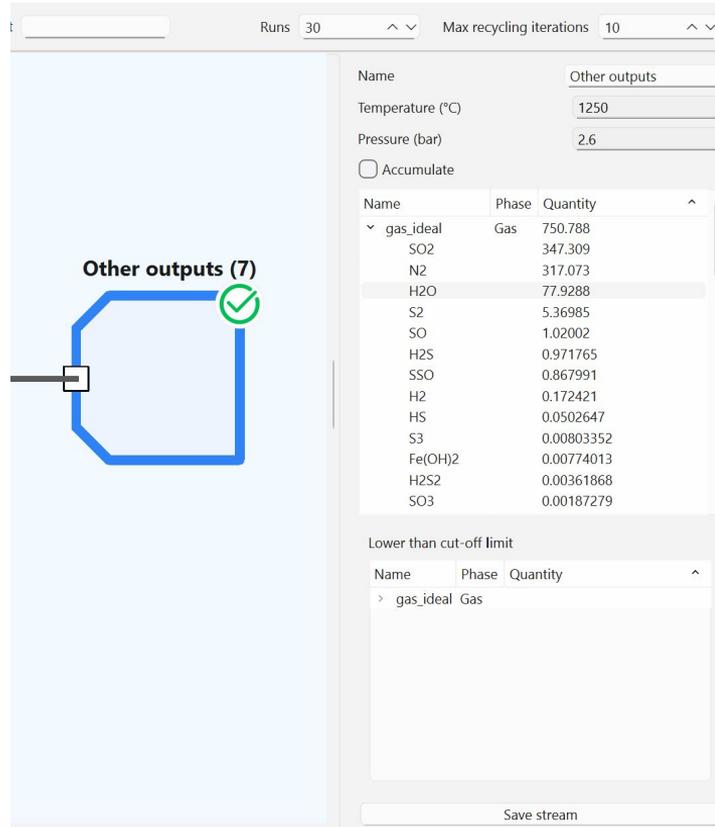
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The **Exit** node is used to view the contents of an output stream in your flowsheet.



Runs: 30 | Max recycling iterations: 10

Name: Other outputs

Temperature (°C): 1250

Pressure (bar): 2.6

Accumulate

Name	Phase	Quantity
gas_ideal	Gas	750.788
SO2		347.309
N2		317.073
H2O		77.9288
S2		5.36985
SO		1.02002
H2S		0.971765
SSO		0.867991
H2		0.172421
HS		0.0502647
S3		0.00803352
Fe(OH)2		0.00774013
H2S2		0.00361868
SO3		0.00187279

Lower than cut-off limit

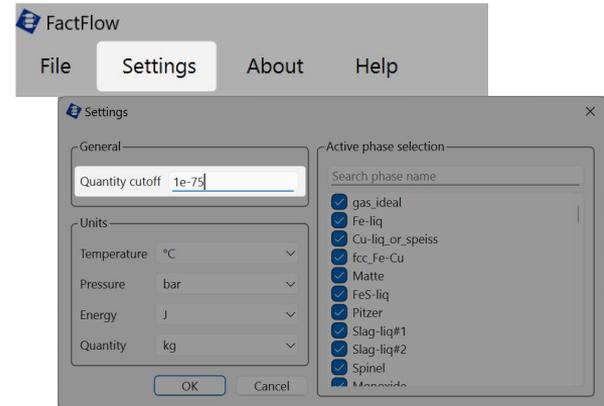
Name	Phase	Quantity
gas_ideal	Gas	

Save stream

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:



FactFlow

File Settings About Help

Settings

General

Quantity cutoff: 1e-75

Units

Temperature: °C

Pressure: bar

Energy: J

Quantity: kg

Active phase selection

Search phase name

- gas_ideal
- Fe-liq
- Cu-liq_or_speiss
- fcc_Fe-Cu
- Matte
- FeS-liq
- Pitzer
- Slag-liq#1
- Slag-liq#2
- Spinel
- Mnoxide

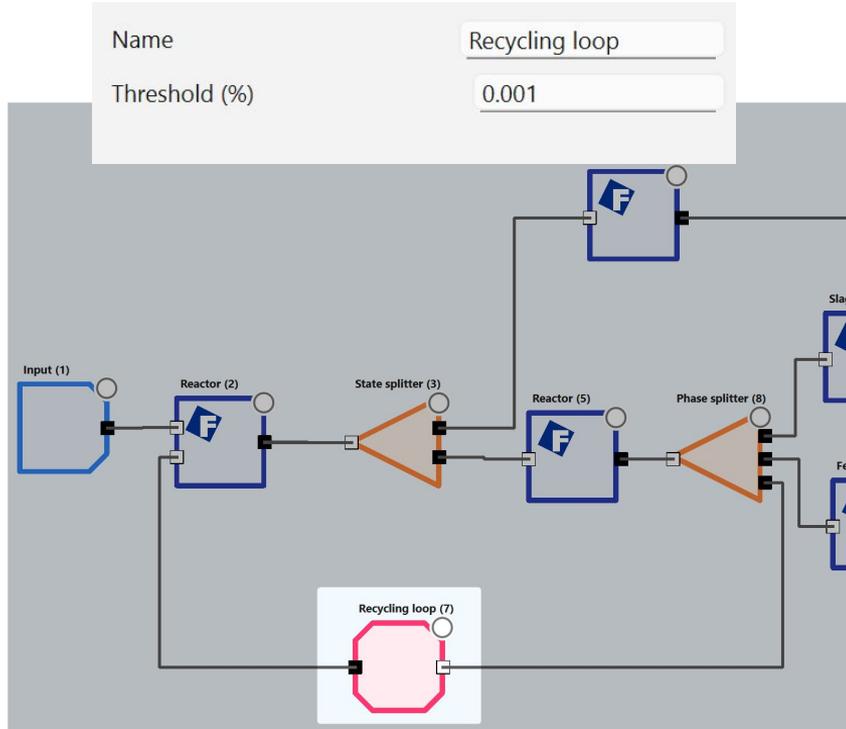
OK Cancel

Accumulate: Sums output values across multiple recycling iterations.

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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.

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

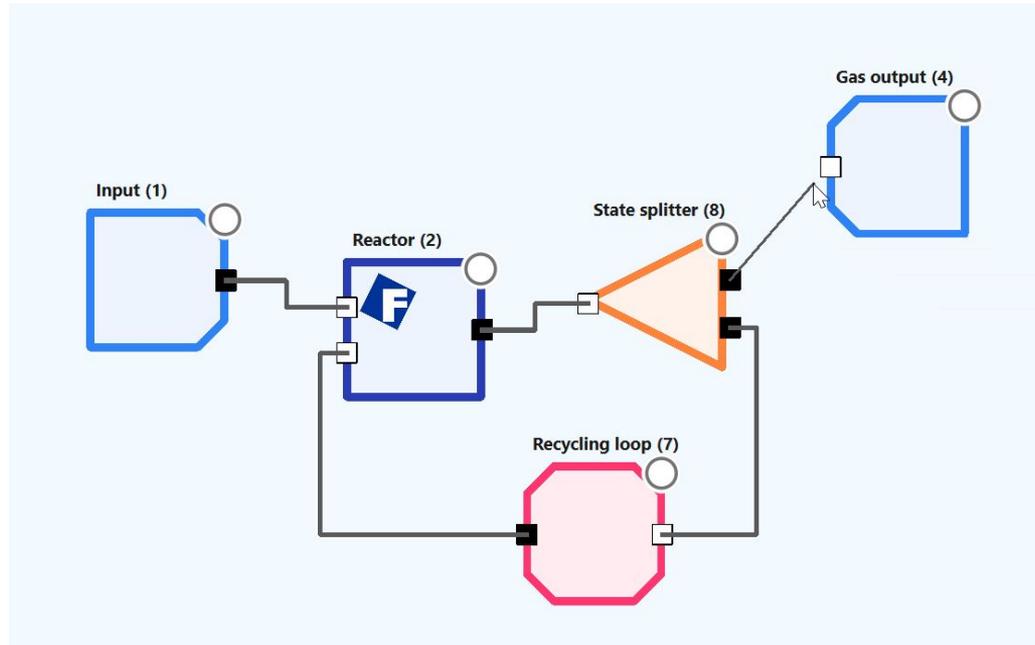
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Build the Flowsheet - Connecting nodes

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

Configure Run Settings

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Understanding Runs vs. Recycling Iterations

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

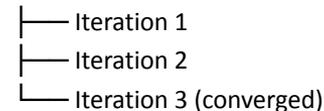
1. Runs (Parametric Runs)

- 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.

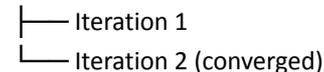
2. Recycling Iterations (Inside each Run)

- 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.

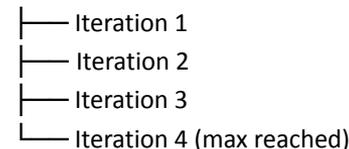
Run 1



Run 2



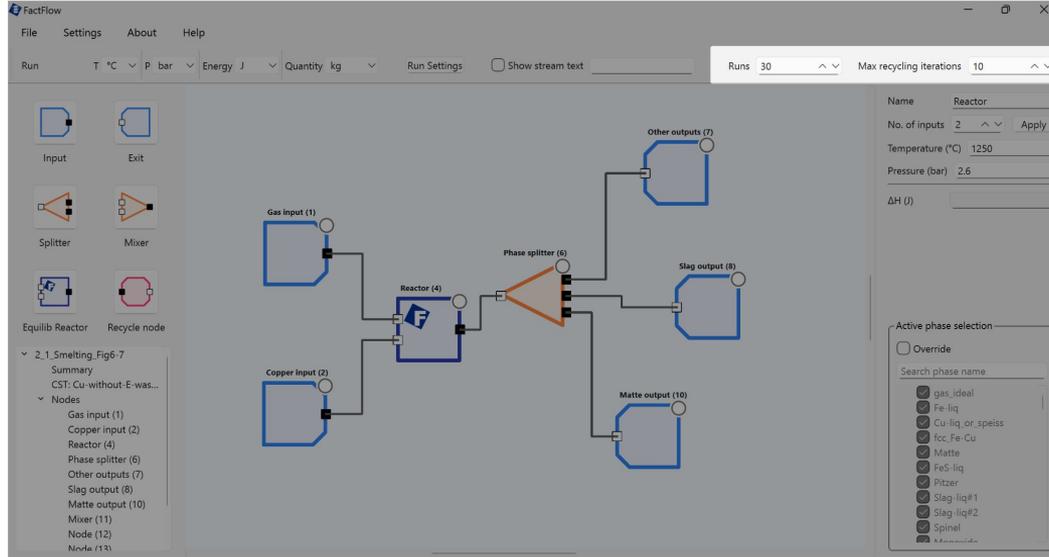
Run 3



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The screenshot shows the FactFlow software interface. The main window displays a flowsheet with several nodes: Gas input (1), Copper input (2), Reactor (4), Phase splitter (6), Other outputs (7), Slag output (8), and Matte output (10). The Run Settings panel is open, showing the following configuration:

- Runs: 30
- Max recycling iterations: 10
- Temperature (°C): 1250
- Pressure (bar): 2.6
- ΔH (J):

The Active phase selection panel is also visible, showing a list of phases with checkboxes:

- Override
- gas_ideal
- Fe_liq
- Cu_liq_or_speiss
- fcc_Fe-Cu
- Matte
- FeS_liq
- Pitzer
- Slag_liq#1
- Slag_liq#2
- Spinel

Set Runs and Max Recycling Iterations

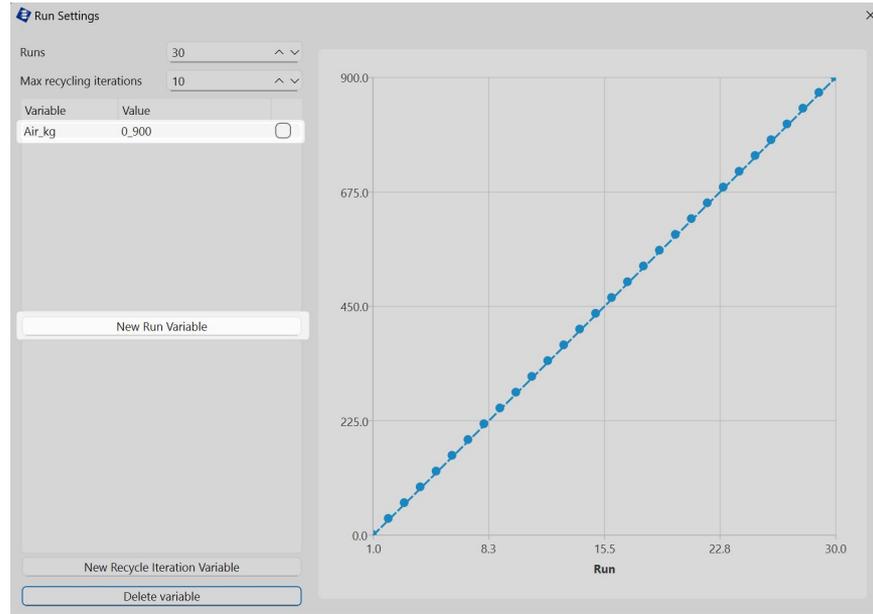
- **Runs** field: Controls how many parametric runs will be executed.
- **Max recycling iterations** field: Controls the maximum number of iterations per run *if* recycling is active.

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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The screenshot shows the 'Run Settings' dialog box. On the left, there are input fields for 'Runs' (30) and 'Max recycling iterations' (10). Below these is a table with two columns: 'Variable' and 'Value'. The table contains one entry: 'Air_kg' with a value of '0_900'. A 'New Run Variable' button is located below the table. At the bottom of the dialog, there are fields for 'New Recycle Iteration Variable' and a 'Delete variable' button. On the right side of the dialog, there is a scatter plot with 'Run' on the x-axis (ranging from 1.0 to 30.0) and 'Air_kg' on the y-axis (ranging from 0.0 to 900.0). The plot shows a series of blue dots connected by a line, forming a straight line that starts at (1.0, 0.0) and ends at (30.0, 900.0).

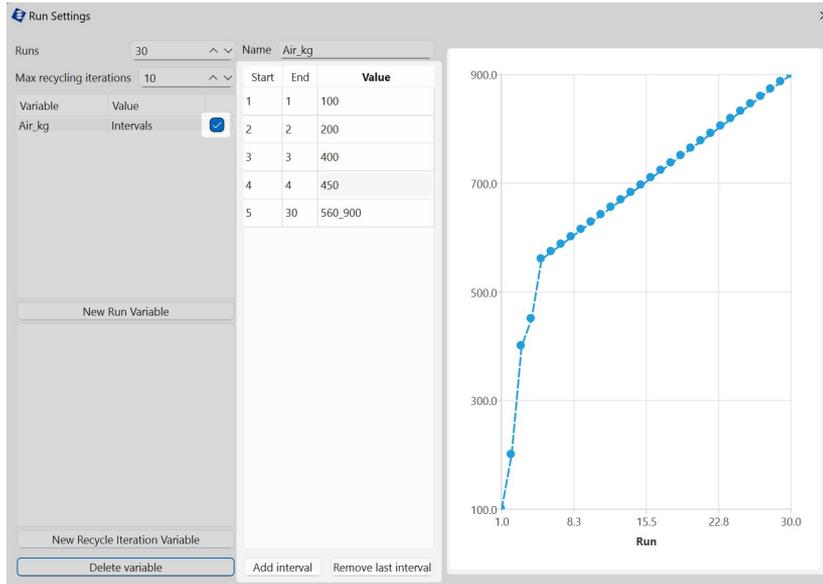
- Click **New Run Variable** to add a variable.
- Enter the variable's name in the field that appears.
- Rename a variable at any time by double-clicking its name in the variable list.
- In the **Value** column, enter a range using the format: **MIN_MAX**
 - Example: 0_900 will vary the value from 0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

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Configure Run Settings - Advanced Intervals

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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.

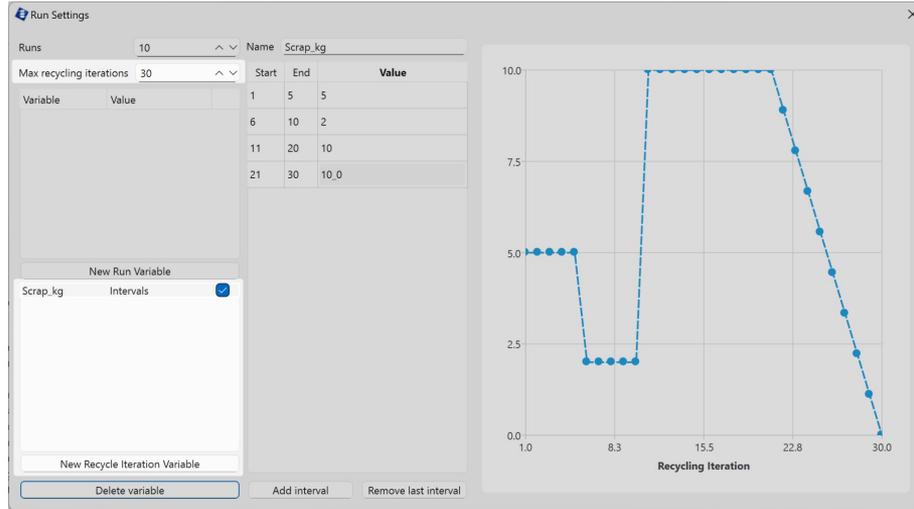
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Configure Run Settings - Recycle Iteration Variables (Advanced)

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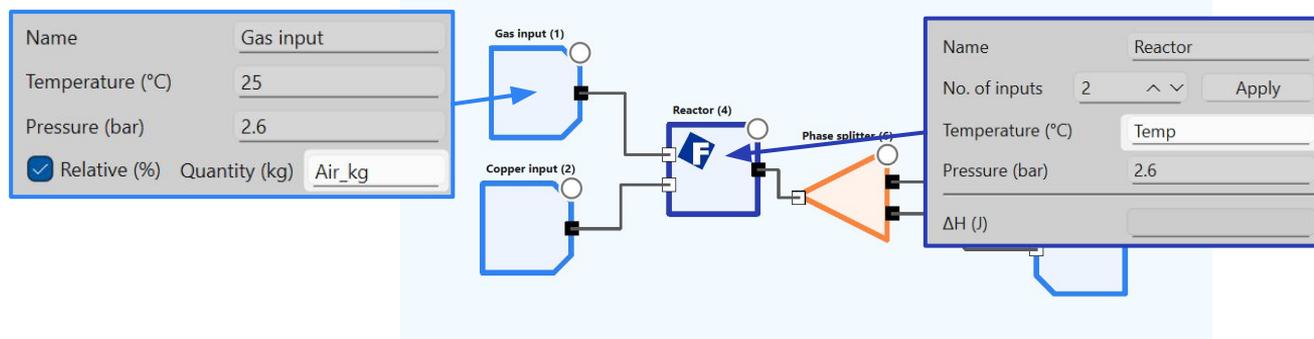
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To use a **Run Variable** or **Recycle Iteration Variable**, simply **type the variable's name into any editable input field** in your flowsheet.

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		

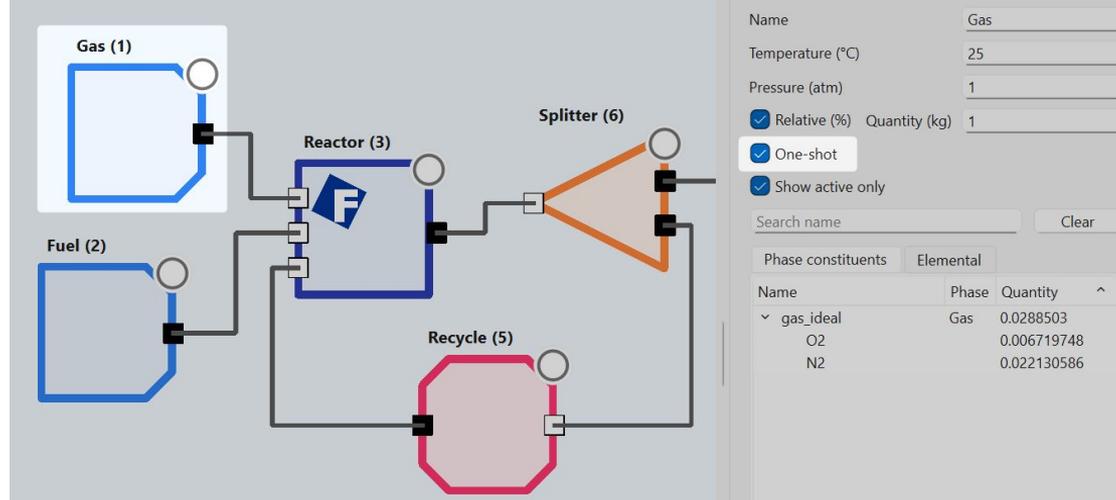
	A	B
1	O2_mol	Purity
2	1	50
3	2	50
4	3	50
5	4	50
6	5	50
7	6	80
8	7	80
9	8	80
10	9	80
11	10	80
12	11	80
13	12	80
14	13	80
15	14	80
16	15	80
17		

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.



The configuration panel for the Gas (1) node is shown on the right. It includes the following settings:

- Name: Gas
- Temperature (°C): 25
- Pressure (atm): 1
- Relative (%) Quantity (kg): 1
- One-shot
- Show active only

The 'Phase constituents' table is also visible:

Name	Phase	Quantity
gas_ideal	Gas	0.0288503
O2		0.006719748
N2		0.022130586

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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:

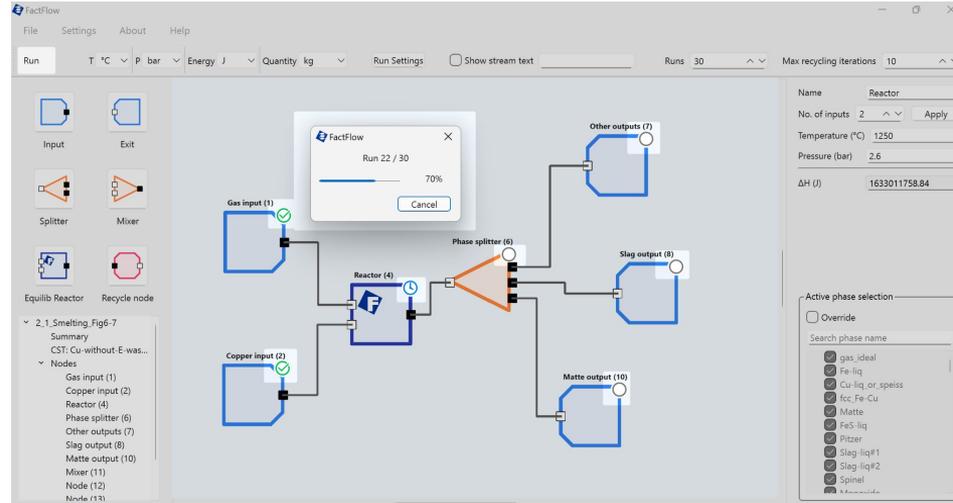
- Launch the simulation using the **Run** button
- Interpret **node status indicators** during execution

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Run the Simulation

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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:

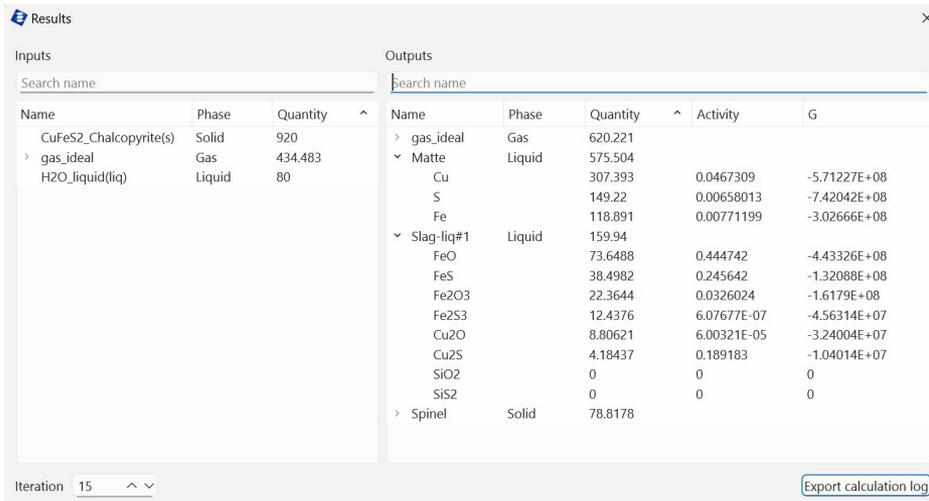
- View **stream results** directly from any node
- Use the **Analysis Module** to generate plots and compare results across runs

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Analyzing Results

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The screenshot shows the 'Results' window with two panels: 'Inputs' and 'Outputs'. The 'Inputs' panel shows a table with columns for Name, Phase, and Quantity. The 'Outputs' panel shows a table with columns for Name, Phase, Quantity, Activity, and G. The 'Iteration' is set to 15, and there is an 'Export calculation log' button at the bottom right.

Inputs			Outputs				
Name	Phase	Quantity	Name	Phase	Quantity	Activity	G
CuFeS2_Chalcocopyrite(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		

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

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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		E+07	
Cu2O	8.80621		E+07	
Cu2S	4.18437	0.169165	-1.04014E+07	
SiO2	0	0	0	
SiS	0	0	0	

- Plot analysis
- Plot elemental analysis

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

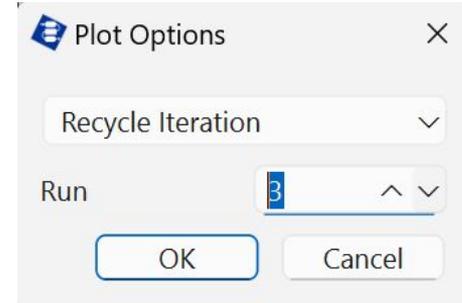
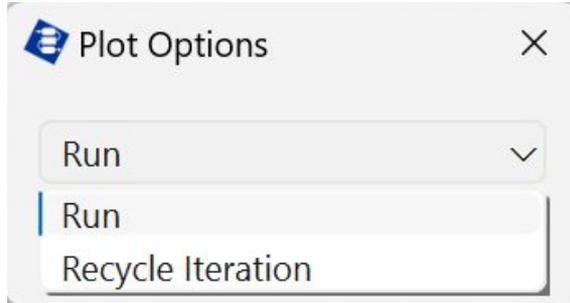
This allows you to customize exactly what gets sent to the **Analysis Module** for plotting.

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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.

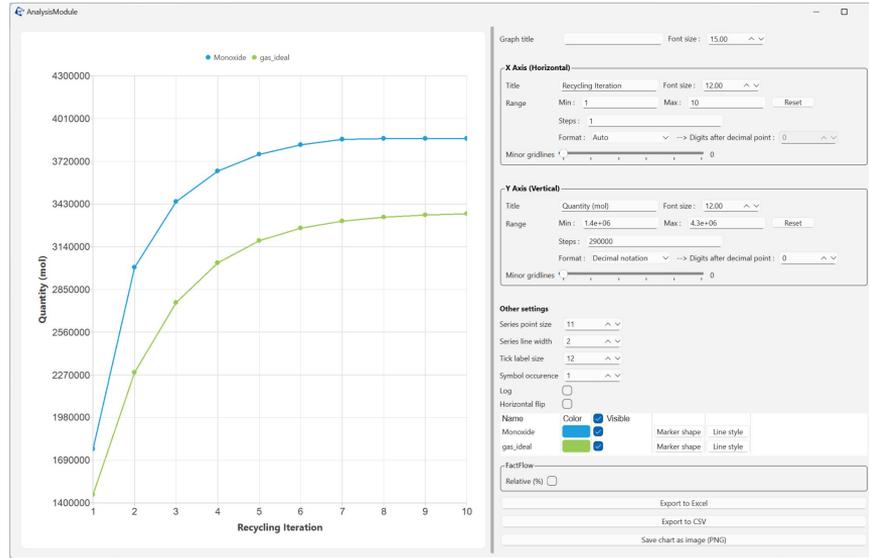
Click **OK** to proceed to the Analysis Module with your selected view.

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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

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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:

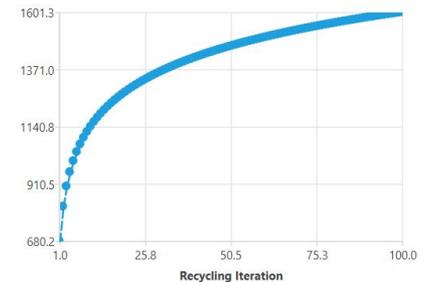
- **Basic arithmetic:** +, -, *, /, ^
- **Parentheses** for grouping: $(A + B) / 2$
- **Math functions:** $\text{sqrt}(x)$, $\text{log}(x)$, $\text{exp}(x)$, $\text{abs}(x)$, $\text{min}(a, b)$, $\text{max}(a, b)$
- **Constants:** pi, e

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

No. of inputs	4	^ v	Apply
Temperature (°C)	<input type="text" value="200*log(i*30)"/>		
Pressure (atm)	<input type="text" value="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

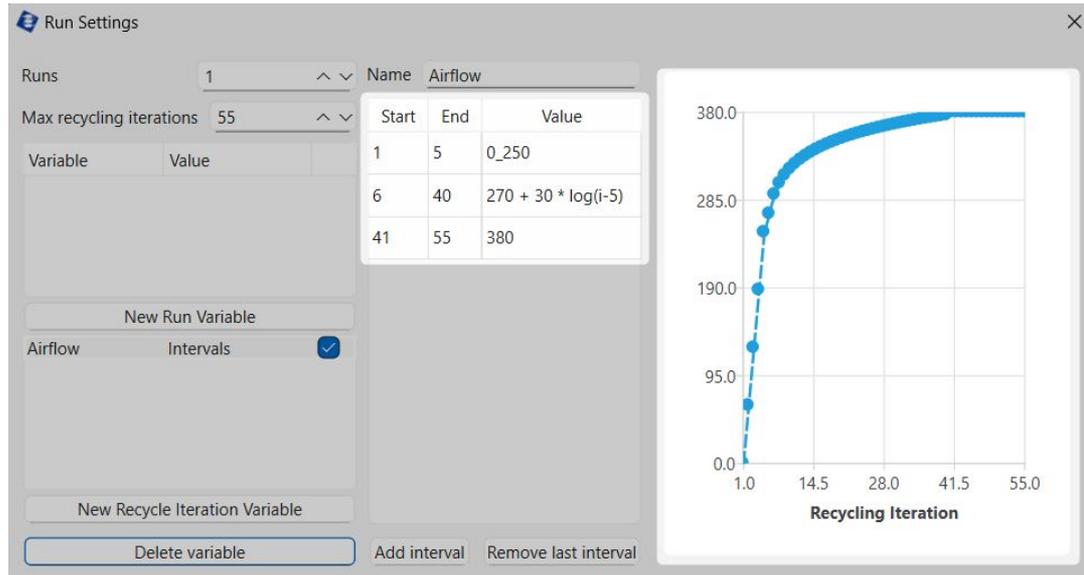
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In addition to input fields, mathematical expressions can also be used in the **Value** column of the Run Settings panel — both in **basic** and **interval** modes.

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:



The screenshot shows the 'Run Settings' window for a simulation. The 'Runs' section is set to 1, and the 'Max recycling iterations' is 55. The 'Airflow' variable is defined with three intervals:

Start	End	Value
1	5	0_250
6	40	$270 + 30 * \log(i-5)$
41	55	380

The graph on the right plots 'Airflow' (Y-axis, 0.0 to 380.0) against 'Recycling Iteration' (X-axis, 1.0 to 55.0). The data points show a sharp initial increase from 0 to approximately 380 within the first 5 iterations, followed by a gradual increase to a steady-state plateau of 380.0 by iteration 41, which remains constant until iteration 55.

This allows you to model:

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

All within a single simulation run.

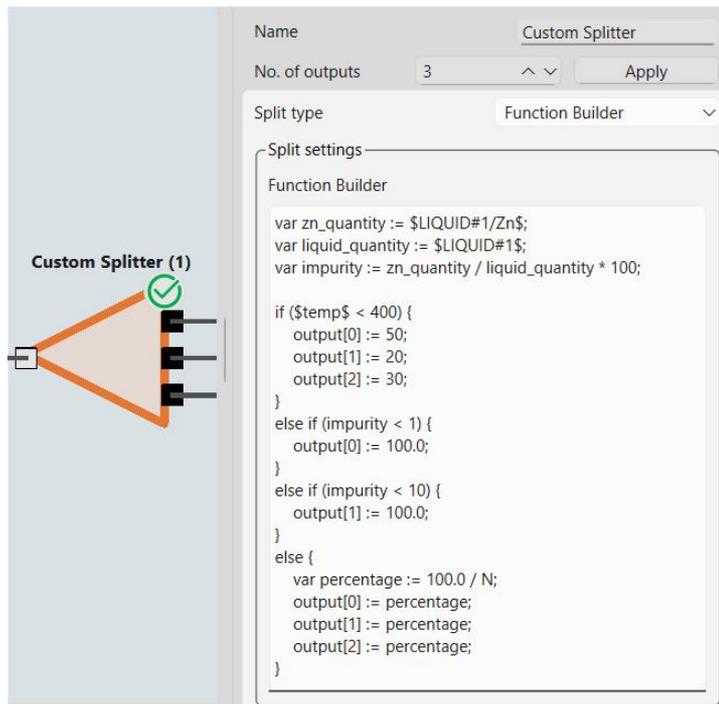
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Function Builder - Splitter

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.



The screenshot shows the configuration for a 'Custom Splitter' node. The 'Split type' is set to 'Function Builder'. The function builder contains the following code:

```

var zn_quantity := $LIQUID#1/Zn$;
var liquid_quantity := $LIQUID#1$;
var impurity := zn_quantity / liquid_quantity * 100;

if ($Temp$ < 400) {
  output[0] := 50;
  output[1] := 20;
  output[2] := 30;
}
else if (impurity < 1) {
  output[0] := 100.0;
}
else if (impurity < 10) {
  output[1] := 100.0;
}
else {
  var percentage := 100.0 / N;
  output[0] := percentage;
  output[1] := percentage;
  output[2] := percentage;
}
    
```

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.

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