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FactProSim

Installation Guide and Program Description June 2024



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FactProSim installation

FactProSim runs on any windows machine with minimal installation and is designed with a drag-and-drop approach to provide an intuitive and user-friendly interface

It is powered by accurate FactSage thermodynamic databases complex, multicomponent, multiphase chemical equilibria and their associated extensive property balances

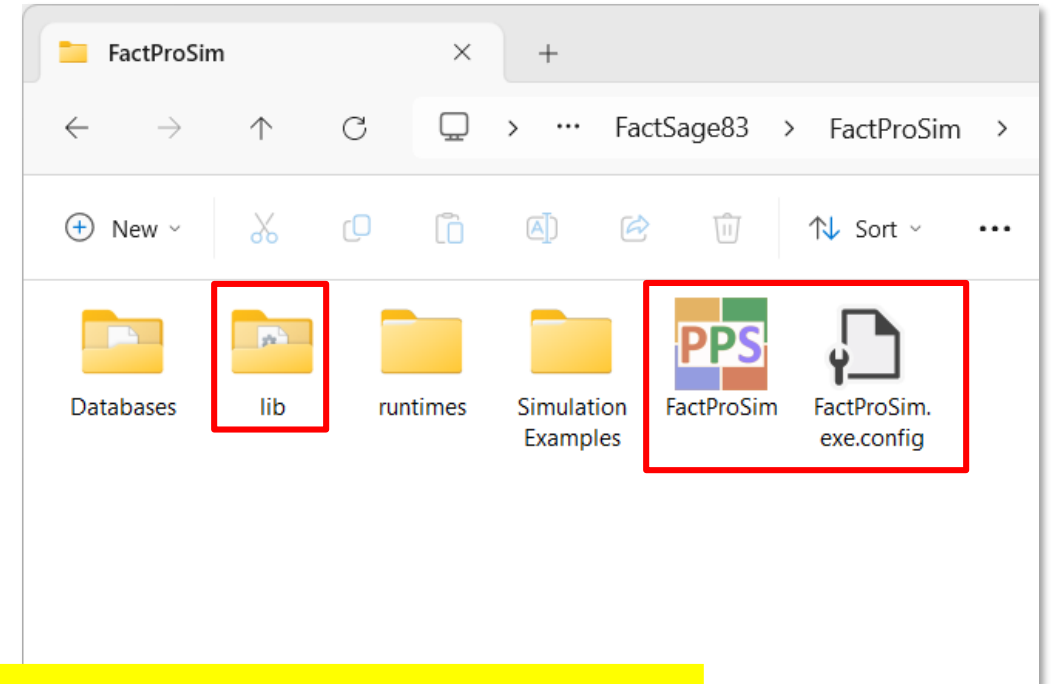
To install FactProSim on your Windows computer,

- 1) Download the FactProSim add-on
- 2) This add-on contains FactProSim folder and ff32.dll, please extract the content and place both of them inside the FactSage folder

Overview of the FactProSim package

The FactProSim package contains 5 items:

1. The Application file *FactProSim.exe*: executable file to start the program
2. The Configuration file *FactProSim.exe.config*, which contains settings to run FactProSim.exe
3. The folder *lib*, which contains all the libraries necessary to run the program FactProSim.exe

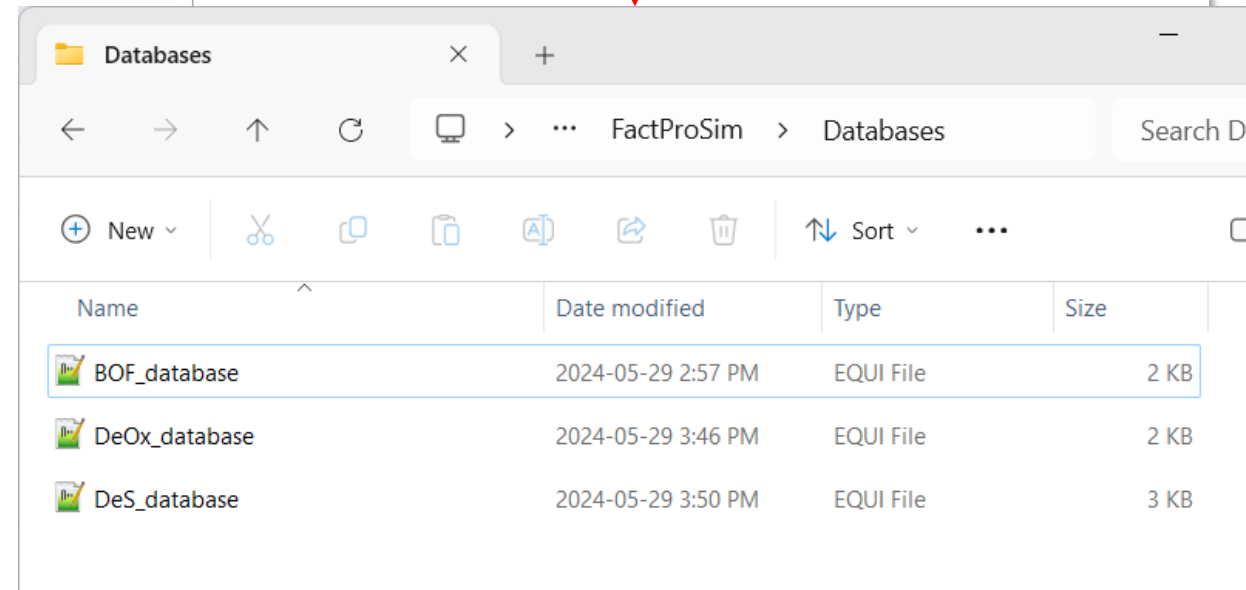
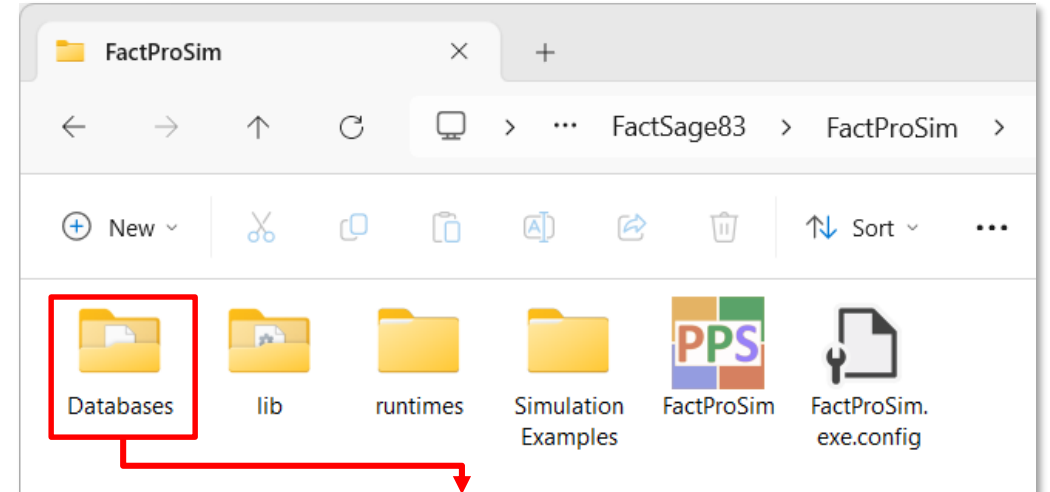


⚠ Do not rename, move or delete these files, this folder and its content! These 3 items are required for the program to run
The folder *lib* AND the file *FactProSim.exe.config* MUST be located in the same folder as *FactProSim.exe*. If not, the program FactProSim won't run

Overview of the FactProSim package

The FactProSim package contains (continued):

4. The folder *Databases*: the folder holds 3 equilb files (*.equi) containing the phase selection to generate the database files (cst files) for the examples

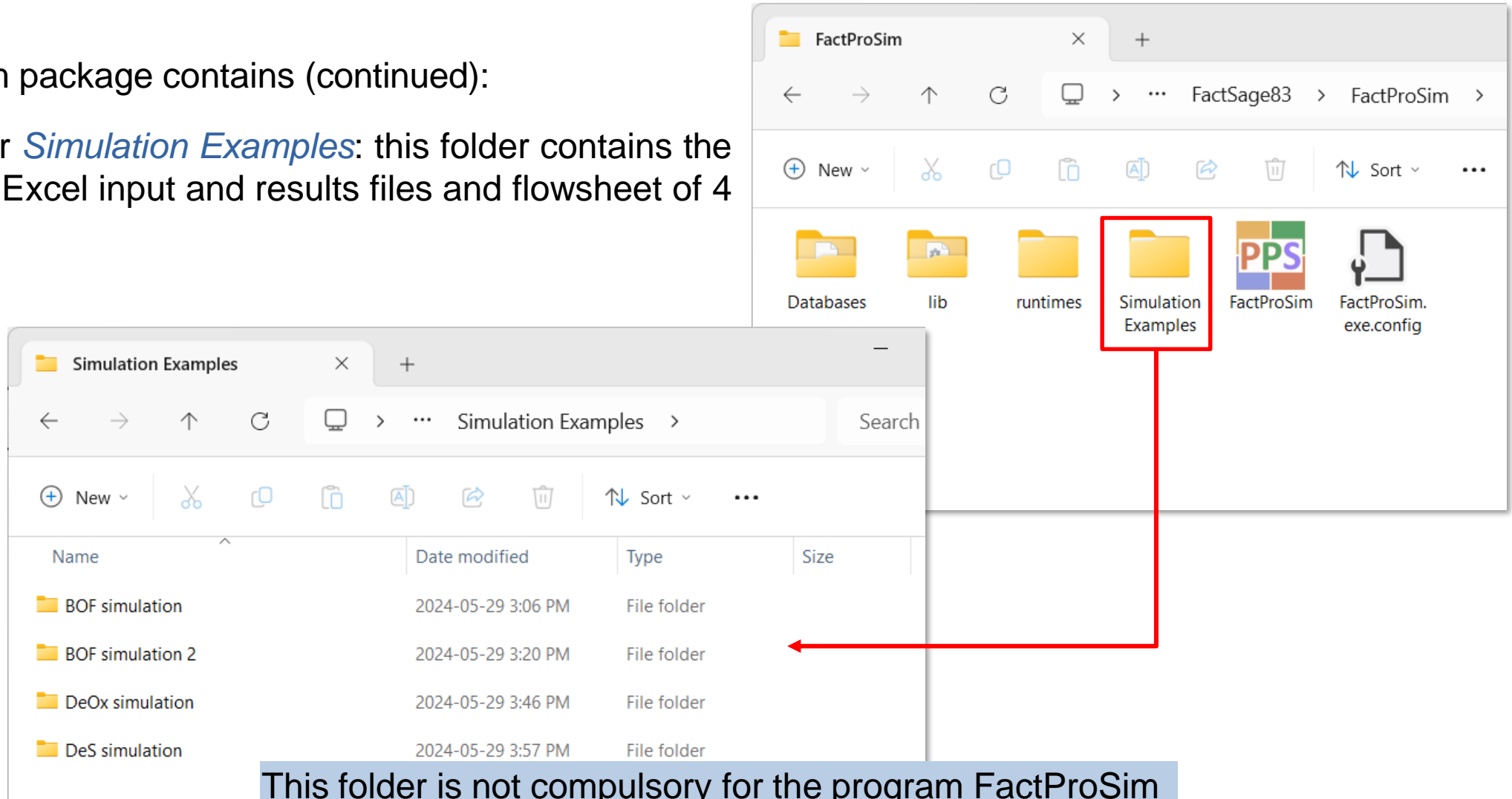


This folder is not compulsory for the program FactProSim to run. It can be modified, moved or deleted by the user

Overview of the FactProSim package

The FactProSim package contains (continued):

5. The folder *Simulation Examples*: this folder contains the description, Excel input and results files and flowsheet of 4 examples



This folder is not compulsory for the program FactProSim to run. It can be modified, moved or deleted by the user

Description of the program

Overview of the main window and commands in the Toolbar

- Step 1: Create and load a database file
- Step 2: Build the Process Flowsheet
 - Modules Panel
 - Input Stream module
 - Splitter module
 - Equilib module
 - Heat Exchanger module
 - Using Excel Links in the modules
- Step 3: Check the modules – The Initializer
- Step 4: Run the process flowsheet
- Step 5: View the Results (Output Excel File)
- Using Equations in the modules
- Transferring material to the next step
- Changing global and local units
- Manage Splitter and Equilib Process IDs
- Align the process modules in the flowsheet
- Save and load an existing flowsheet

Overview of the Main Window

The screenshot shows the FactProSim software interface. The title bar reads "FactProSim" and includes standard window controls. The menu bar contains "New", "Save", "Load", "Steps" (with a value of 1), "Run", "Units", "CST", "Stop", "About", and "Help".

On the left side, there are three panels:

- Modules Panel:** Contains icons for "Input Stream", "Stream", "Splitter", "Equilib", and "Heat Ex".
- Arrange Panel:** Contains icons for "Align Vertical" and "Align Horizontal".
- Extra Tools:** Contains icons for "Excel Files", "Initializer", and "Rearrange Process IDs".

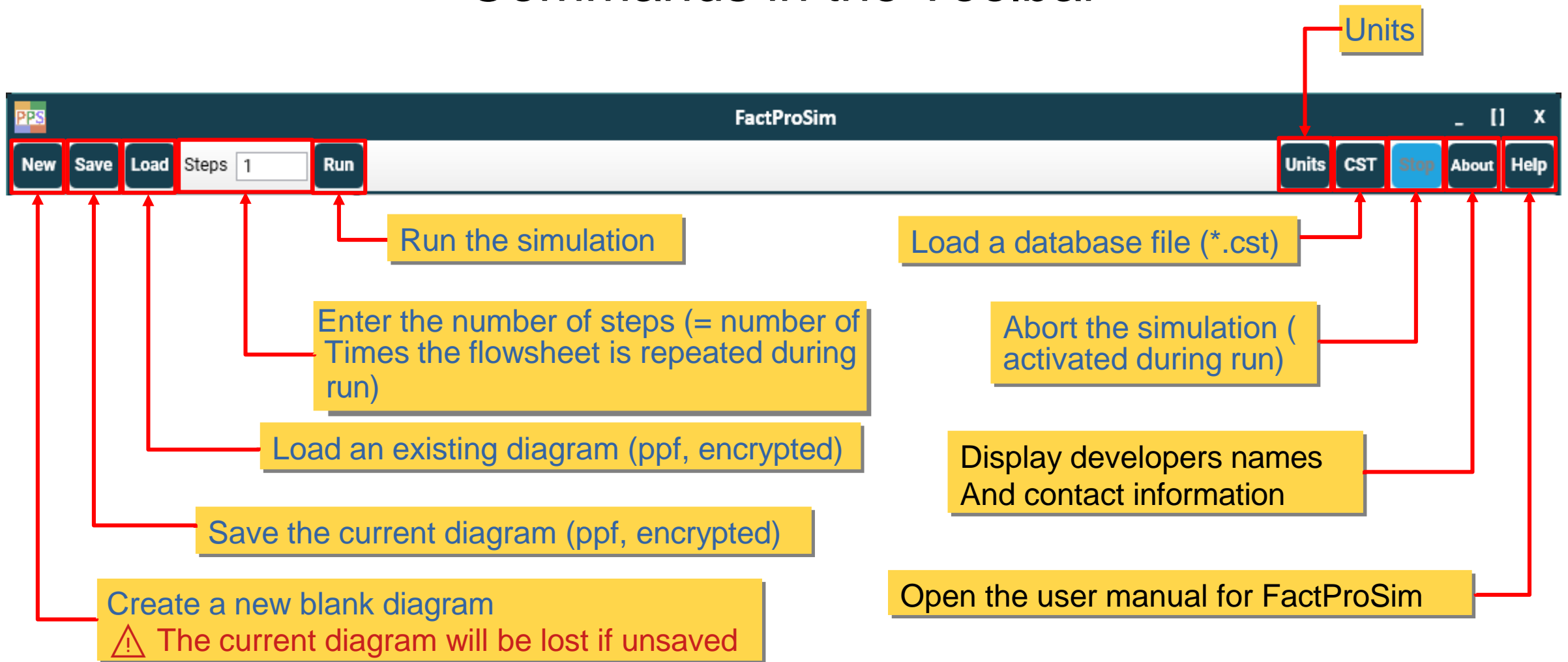
The main workspace is titled "Unsaved*" and displays a diagram (flowsheet). At the top of the workspace, there are "Zoom and view controls" including a play button and a slider set to "100 %".

Callouts with arrows point to the following elements:

- Toolbar:** Points to the menu bar.
- Modules Panel:** Points to the Modules section of the left sidebar.
- Arrange Panel:** Points to the Arrange section of the left sidebar.
- Extra Tools:** Points to the Tools section of the left sidebar.
- Zoom and view controls:** Points to the slider and play button in the workspace.
- Diagram (flowsheet) Workspace:** Points to the main workspace area.

At the bottom left, the version number "Version: 2.1.8909" is displayed.

Commands in the Toolbar




Zoom and view controls

The screenshot displays the FactProSim software interface. At the top, there is a menu bar with 'New', 'Save', 'Load', 'Steps' (set to 45), 'Run', 'Units', 'CST', 'Step', 'About', and 'Help'. Below the menu bar, there are three panels: 'Modules' (containing Input Stream, Stream, Splitter, Equilib, and Heat Ex), 'Arrange' (containing Align Vertical and Align Horizontal), and 'Tools' (containing Excel Files, Initializer, and Rearrange Process IDs). The main workspace, titled 'LF2023_new', features a zoom bar at the top with a slider set to 100%. A flowsheet diagram is shown below, consisting of several interconnected process blocks: 'AIC', '1', 'AIC comb', '2', 'disolv AIC', 'Undisolv A', and '3'. A red arrow points from the zoom bar to the 'FeTi' block, and another red arrow points from the 'FeTi' block to the '7' block. A yellow callout box is overlaid on the right side of the interface, containing two paragraphs of text.

You can adjust the zoom level of the flowsheet workspaces by moving the slider of the zoom bar

Alternatively, the zoom level can also be changed by holding the "CTRL" key and rolling the scroll wheel on your mouse upwards or downwards

Zoom and view controls (continued)

The Zoom bar can be repositioned anywhere in the flowsheet Workspace by dragging the bar when the moving  cursor appears

Press the arrow on the zoom bar to expand or collapse the Navigation tool. It is designed to move easily around the flowsheet when the zoom is set higher than what the diagram workspace can display

The rectangle shows the location of the current view in the diagram

Click and drag the rectangle to change the location of the current view

General behavior in windows

Input Stream

Local Units

Name: FeTi

Temperature (C) Check Sched:

Amount (g) Check Sched:

Pressure (atm) Check Sched:

Components ADD

Mass Percent	Species
0.4	N
0.2	C
0.006	S
0	Mg
4.5	Al
0.21	Si
0.01	P

Total%: 100

OK Schedule

Press the 'X' button in the title bar to close the Window **without applying (saving) the changes** (= Cancel button, reverts back to original)

Press OK to close the window and **apply (save) the changes**

If errors are found (invalid or missing entries) in the module window, the program will display a message and the window will not close

General behavior in windows

The screenshot displays the 'Input Stream' window in FactProSim. The window title is 'Input Stream' with a close button (X) in the top right corner. Below the title bar, there is a 'Local Units' section and a 'Description:' text field. The main area is divided into sections for 'Excel Link Equation', 'Gas Phase Species', 'Solution Phases', and 'Pure Solids'. The 'Name' field contains 'FeTi'. There are several 'Check Sched' toggle buttons for Temperature (C), Amount (g), and Pressure (atm). A 'Components' section has an 'ADD' button and a list of species with their mass percents. A list of species is also shown on the right side of the window. At the bottom of the window, there are 'OK' and 'Cancel' buttons.

A yellow callout box highlights the 'Description:' field with the text: "The Description field is used to make comments about the window and this comment will be shown on the flowsheet outside".

Overlaid on the bottom right is a process flow diagram. It shows a process flow starting with an 'Input Stream' module (represented by an orange square with a plug icon) labeled 'FeTi'. This module is connected to an 'Equilib' module (represented by an orange square with a double arrow icon). The 'Equilib' module is connected to a 'Heat Ex' module (represented by a red square with a circular arrow icon). The 'Heat Ex' module is connected to a '7' module (represented by a red square with a double arrow icon). The 'Input Stream' module has a label 'Input FeTi' below it. The 'Equilib' module has a label 'Equilib' below it. The 'Heat Ex' module has a label 'Heat Ex' below it. The '7' module has a label '7' above it. The diagram also shows a 'Modules' palette with icons for 'Input Stream', 'Stream', 'Splitter', 'Equilib', and 'Heat Ex'. Below the palette is an 'Arrange' section with 'Align Vertical' and 'Align Horizontal' options. A 'Steps' field is set to '45' and a 'Run' button is visible. A 'Unsaved*' status bar and a '100%' zoom slider are also present.

Working on flowsheets


- Create a new flowsheet from the start (blank Diagram Workspace)

The screenshot shows the FactProSim software interface. The title bar reads 'FactProSim'. The toolbar contains buttons for 'New', 'Save', 'Load', 'Steps' (with a value of 1), 'Run', 'Units', 'CST', 'Stop', 'About', and 'Help'. The 'New' button is highlighted with a red box. Below the toolbar, there are two panels: 'Modules' and 'Arrange'. The 'Modules' panel contains icons for 'Input Stream', 'Stream', 'Splitter', 'Equilib', and 'Heat Ex'. The 'Arrange' panel contains icons for 'Align Vertical' and 'Align Horizontal'. A yellow callout box points to the 'New' button with the text: 'Click the button 'New' in the toolbar to clear the Diagram Workspace of all modules'. In the foreground, a dialog box titled 'New Flowsheet?' is displayed. It features a yellow warning triangle icon and the text: 'Clear the current flowsheet? Unsaved changes to the current flowsheet will be lost'. At the bottom of the dialog are 'Yes' and 'No' buttons. A yellow callout box points to the dialog with the text: 'The program prompts to clear the current flowsheet' and 'Click Yes to clear or No to cancel and return to the current flowsheet'.

Working on flowsheets (continued)

Work on an existing flowsheet:

- Using the AutoSave flowsheet. This flowsheet is an automatically-saved copy of the flowsheet in the Diagram Workspace when the user exited the program properly during the last session. When starting the program, if an AutoSave file exists (i.e. user was working on flowsheet previously) the program prompts to restore the previous session, and if allowed then the AutoSave flowsheet is loaded to easily take up where the user left off. As the AutoSave file is also updated after main changes in the flowsheet, some unsaved work can be recovered in case of a sudden crash of the program
- Using an existing flowsheet saved in a file by the user. The saved flowsheet can be opened in the Diagram Workspace using the [Load command](#)

 AutoSave does not replace the [Save command](#). You should use The Save command to save the flowsheet at regular intervals and when You finish working on it

Description of the program

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 - Heat Exchanger module
 - Using Excel Links in the modules
 - Using Equations in the modules
 - Transferring material to the next step
 - Changing global and local units
 - Manage Splitter and Equilib Process IDs
 - Align the process modules in the flowsheet
 - Save and load an existing flowsheet
- Step 3: Check the modules – The Initializer
- Step 4: Run the process flowsheet
- Step 5: View the Results (Output Excel File)

Step 1: Create a database file

FactProSim utilizes 'transparent' ChemSage file (*.cst file), which is a thermochemical data file to store the thermodynamic properties of the phases to be included in the flowsheet. In other words, these cst files are a subset of the large commercial and private databases included in FactSage

These thermochemical data cst files can be created with the Equilib module of FactSage, either

- From an entered reactants list and phases selection
- From an existing *.equi file

Step 1: Create a database file

➤ From reactants and phase selection

Equilib - Reactants

File Edit Run Macro Table Units Data Search Data Evaluation Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Quantity(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
1	Fe				1	
+ 1	C				1	
+ 1	Si				1	
+ 1	CaO				1	
+ 1	SiO2				1	
+ 1	MnO					

1. Enter the desired reactants in the reactants window.
Note that the species and the quantities are not important. Make sure that all desired elements are listed

FactSage 8.3 Compound: 3/27 databases Solution: 2/24 databases

Data Search - Equilib 8.3

Databases - 3/27 compound databases, 2/24 solution databases

Fact FactSage[®] SGTE

FactPS FSopp BINS CON2 CON4 CUTE

FToxid FSlead SGPS Coke FELQ SGTEa

FTsulf FSstel SGTE SGTEb STSC WATE

FTsalt FSupsi SGsold

FTmisc

FTball

FToxCN

FTfritz ELEM SGnobl

FThelp SpMCBN

FTpulp FTlite TDmeph

FTdemo FTnucl TDnucl

Private Databases

compounds only
solutions only
no database

Clear All

Add/Remove Data

RefreshDatabases

Information -

Options - search for products

Default

Include

gaseous ions (plasmas)

aqueous species

limited data compounds (25C)

Organic species CxHy... X(max) = 2

Minimum solution components: 1 2 cpts

Cancel Summary ... OK

2. Select the desired databases (both commercial and private databases can be selected)

Step 1: Create a database file

➤ From reactants and phase selection

Equilib - Menu: last system

File Units Parameters Help

T(C) P(atm) Energy(J) Quantity(g) Vol(litre)

Reactants (6)

(gram) Fe + C + Si + CaO + SiO2 + MnO

Products

Compound species

gas ideal real 0

aqueous 0

pure liquids 0

* pure solids 46

* - custom selection species: 46

Solution phases

*	+	Base-Phase	Full Name
	<input checked="" type="checkbox"/>	FTmisc-FeLQ	Fe-liq
	<input checked="" type="checkbox"/>	FToxid-SLAGA	A-Slag-liq all oxides + S
		FToxid-SLAGD	D-Slag-liq with CO3
		FToxid-SLAG?	?-Slag-liq
	<input checked="" type="checkbox"/>	FToxid-SPINB	B-Spinel
		FToxid-SPINC	C-Spinel
		FToxid-SPIN?	?-Spinel
	<input checked="" type="checkbox"/>	FToxid-MeO_A	A-Monoxide

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) 89

Total Solutions (max 200) 5

Total Phases (max 1500) 51

Legend

! - immiscible 1

+ - selected 3

species: 43

solutions: 5 Select

Final Conditions

<A> T(C) P(atm) Product H(J)

1000 1

10 steps Table 1 calculation

Equilibrium

normal normal + transitions

transitions only open

- no time limit - Calculate >>

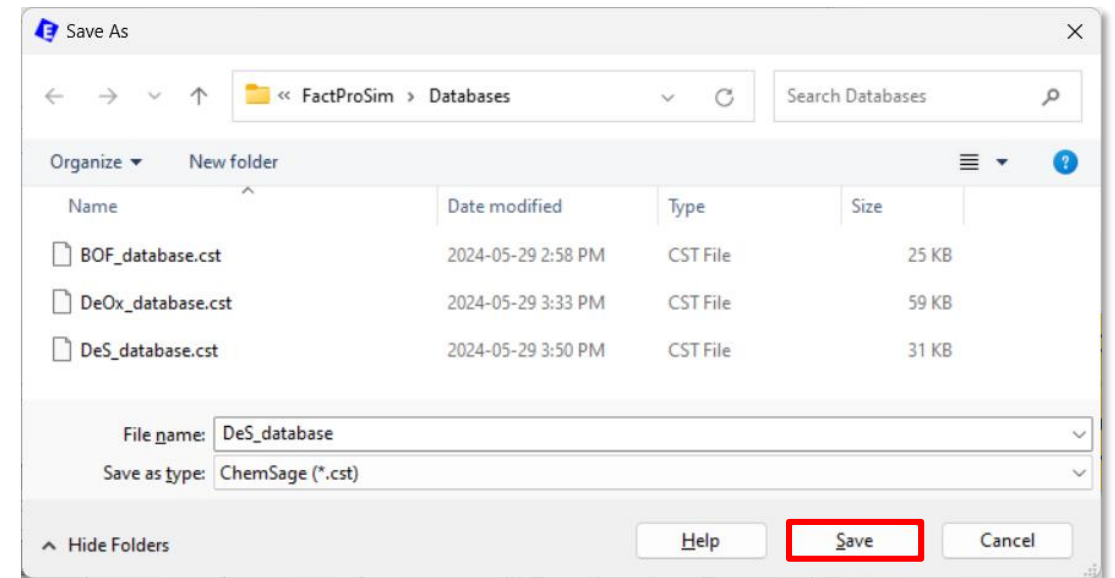
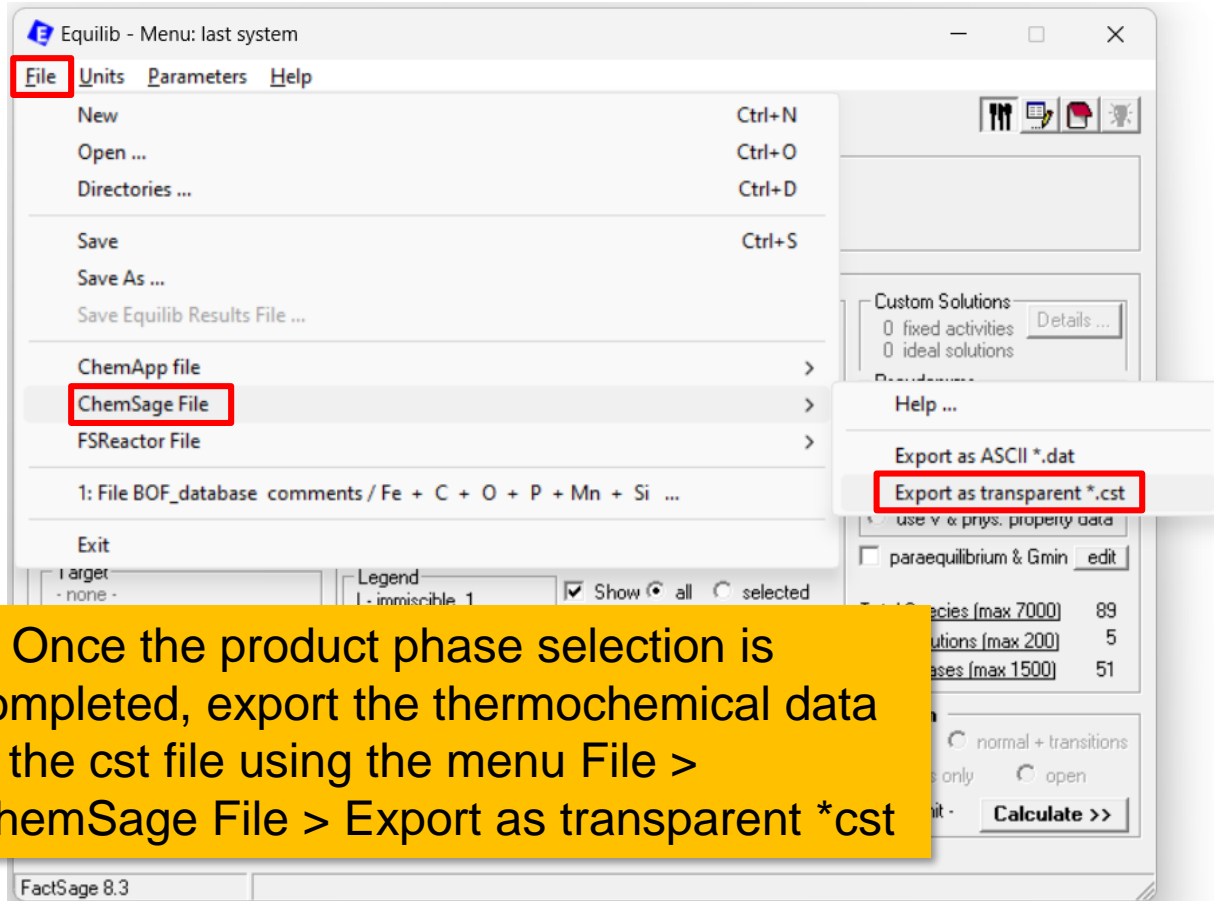
FactSage 8.3

3. Select the product compound species (gas, pure liquids and pure solids) and solution phases

- Final conditions and calculations are not required
- Make sure to select all the desired phases to be stored in the cst file

Step 1: Create a database file

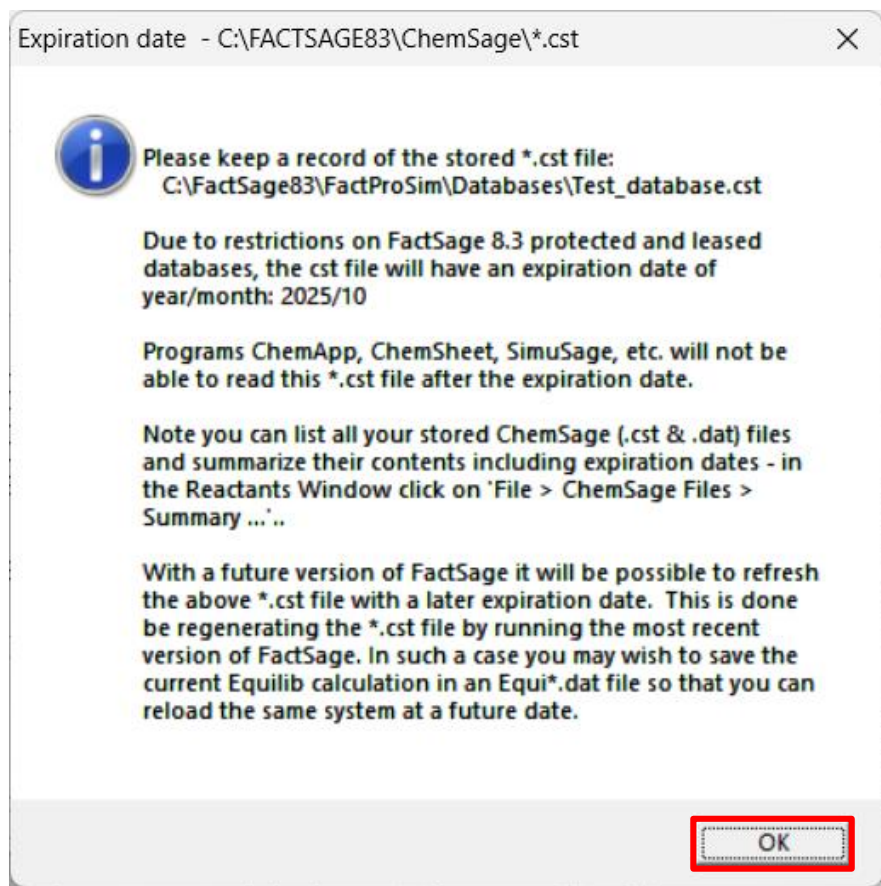
➤ From reactants and phase selection



5. Choose the location and name for the cst file

Step 1: Create a database file

➤ From reactants and phase selection



6. The cst files have an expiration date set by FactSage, after which the file will not be readable by FactProSim (and other ChemApp-based programs)

It is strongly recommended to save the equilib file (*.equi) containing the phase selection to be able to easily regenerate the cst file with FactSage after the expiration date

Step 1: Create a database file

➤ From an existing equilib (*.equi) file

The cst files can be easily generated from an existing Equilib (*.equi) file
To generate the cst file with FactSage, open FactSage and start the Equilib module
In the Equilib module, click on the icon open

The screenshot displays the FactSage 8.3 software interface. The main window is titled 'Equilib - Reactants' and shows a menu bar with 'File', 'Edit', 'Run Macro', 'Table', 'Units', 'Data Search', and 'Data Evaluation'. Below the menu bar, there are several icons, including a folder icon which is highlighted with a red box. A red arrow points from this icon to a file directory window titled 'Directory Equilib (My Files) - D:\...\Alalloy_casting.equi'. This window shows a list of files with columns for 'File', 'Date', and 'Description'. The file 'Alalloy_casting' is selected, with a date of '02Dec21' and a description of 'comments / 90.3 Al + 7 Si + 0.5 Mg + 0.1 Fe + Cu + Zn + 0.1 Mn'. The FactSage 8.3 interface also shows a sidebar with 'Calculate' options, including 'Equilib', which is highlighted with a red box. The status bar at the bottom indicates 'FactSage 8.3 Compound: 1/20 databases Solution: 1/18 databases'.

File	Date	Description
Alalloy_casting	02Dec21	comments / 90.3 Al + 7 Si + 0.5 Mg + 0.1 Fe + Cu + Zn + 0.1 Mn

Step 1: Create a database file

➤ From an existing equilib (*.equi) file

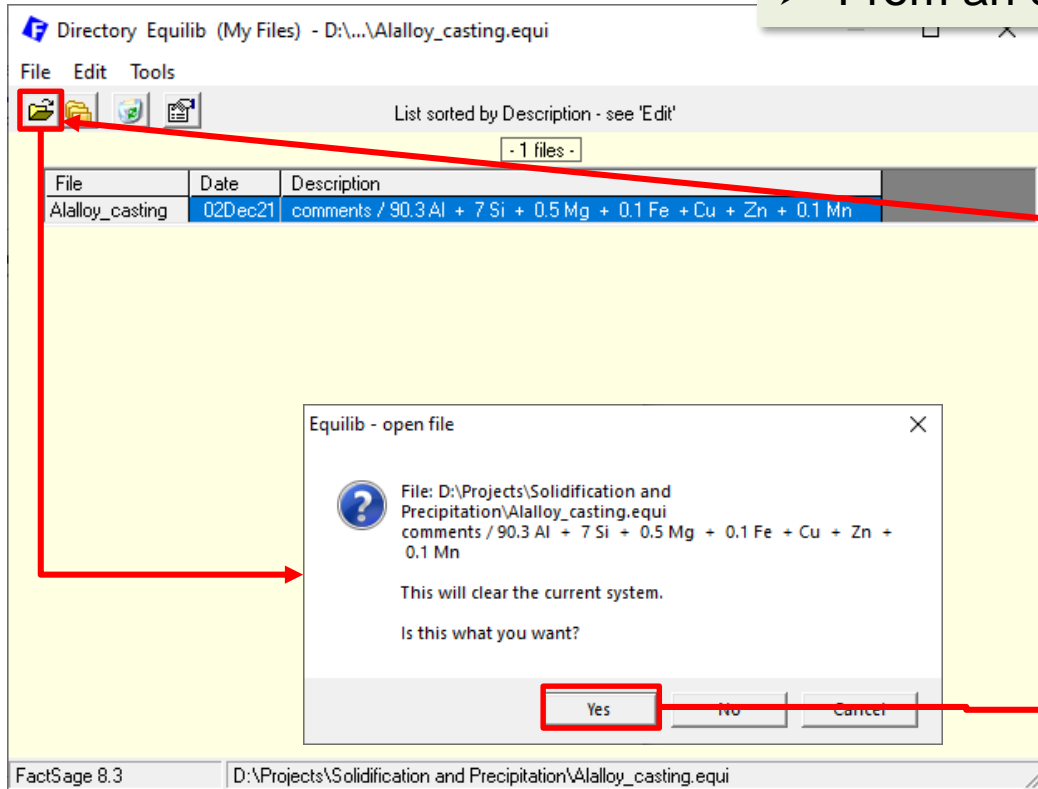
The image shows a sequence of three windows from the FactProSim software. The top window is the 'Directory Equilib' window, displaying a table with one file: 'Alalloy_casting' with a date of '02Dec21' and a description of 'comments / 90.3 Al + 7 Si + 0.5 Mg + 0.1 Fe + Cu + Zn + 0.1 Mn'. A red box highlights the 'Change directory' icon in the toolbar. The middle window shows the 'File' menu with 'Change My Files Directory...' selected, and a red arrow points from this menu item to the 'My Files Directory' dialog box on the right. The dialog box shows the drive 'c:' and a directory tree where 'Solidification and Precipitation' is selected. The file 'Alalloy_casting.equi' is listed in the right pane, and the 'OK' button is highlighted with a red box. A text box at the bottom left provides instructions for this step.

If the desired equilib file is not listed, click on the 'Change directory' icon and choose 'Change My Files Directory...'

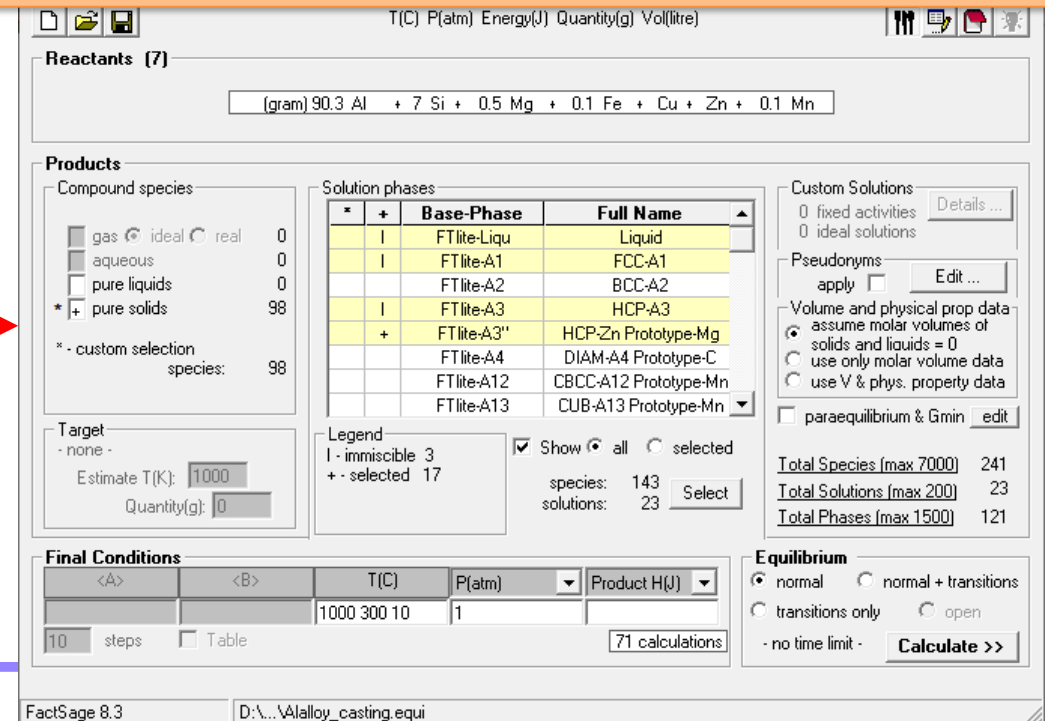
The 'My Files Directory' dialog window opens. Browse the directories and select the desired folder where the *.equi file is located. Click 'OK'

Step 1: Create a database file

➤ From an existing equilib (*.equi) file



Select the desired .equi file in the list
Double-click or select the icon 'Open' to load the equilib file in the Equilib module
Click 'Yes' in the dialog box to clear the current system and load the one saved in the file



Step 1: Create a database file

➤ From an existing equilib (*.equi) file

The screenshot shows the Equilib software interface. The 'File' menu is open, and the 'ChemSage File' option is highlighted with a red box. A red arrow points from the 'ChemSage File' option to the 'Export as transparent *.cst' option, which is also highlighted with a red box. The interface displays various settings for a simulation, including reactants, products, solution phases, and final conditions.

Reactants (7): (gram) 90.3 Al + 7 Si + 0.5 Mg + 0.1 Fe + Cu + Zn + 0.1 Mn

Products: Compound species: gas (ideal/real), aqueous, pure liquids, pure solids, custom selection species.

Solution phases:

*	+	Base-Phase	Full Name
	I	FTlite-Liqu	Liquid
	I	FTlite-A1	FCC-A1
		FTlite-A2	BCC-A2
	I	FTlite-A3	HCP-A3
	+	FTlite-A3''	HCP-Zn Prototype-Mg
		FTlite-A4	DIAM-A4 Prototype-C
		FTlite-A12	CBCC-A12 Prototype-Mn
		FTlite-A13	CUB-A13 Prototype-Mn

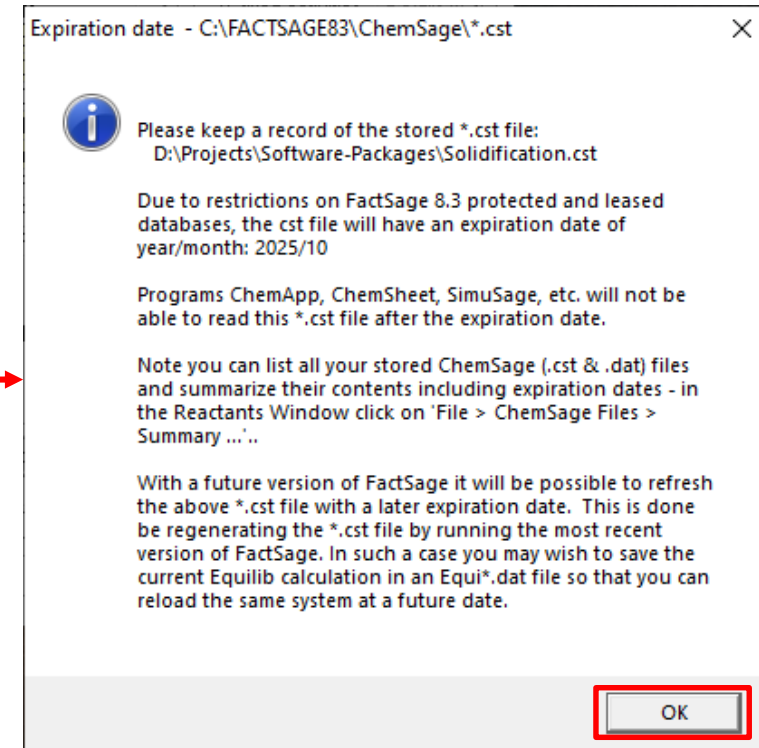
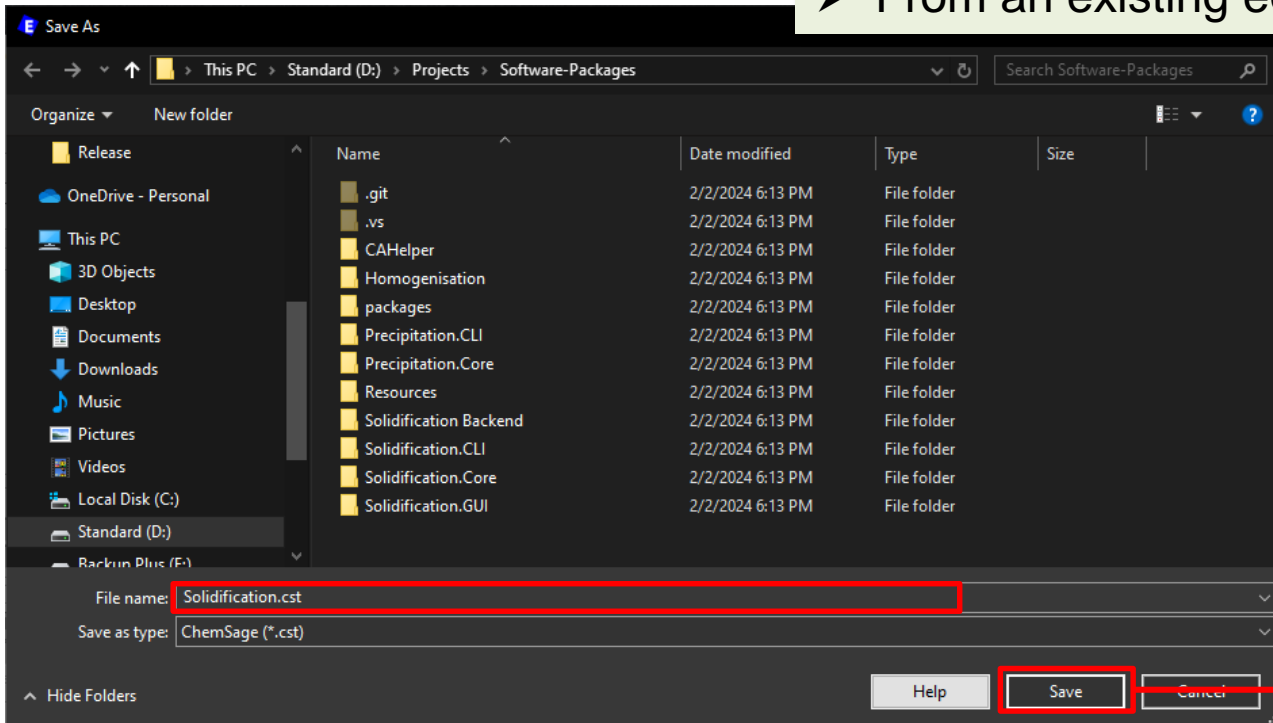
Final Conditions: T(C) 1000, P(atm) 1, Product H(J) 10, 71 calculations.

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

To generate the *.cst file for FactProSim, go to the menu window of Equilib. In the 'File' menu, select 'ChemSage File', then 'Export as transparent *.cst'

Step 1: Create a database file

➤ From an existing equilib (*.equi) file



It will open a save dialog window, where the location and name of the cst file can be entered. Click "Save"

⚠ Because cst files have an expiration date, it is wise to save the original equilib file to be able to regenerate the cst file after the expiration date

Step 1: Load a database file

The first step in designing a flowsheet is to **select a database file** to have appropriate phases to select in the modules

Click the button 'CST' to view and change the current database file (*.cst)

The screenshot shows the software interface with a menu bar containing 'New', 'Save', 'Load', 'Steps', '1', and 'Run'. A toolbar below the menu bar includes 'Units', 'CST', 'Stop', 'About', and 'Help'. The 'CST' button is highlighted with a red box. An 'Open' file dialog is open, showing a list of database files:

Name	Date modified	Type	Size
BOF_database.cst	02-09-2021 14:58	CST File	261 KB
FeMn_database.cst	03-09-2023 23:34	CST File	571 KB
LadleMetall_database.cst	01-07-2021 16:21	CST File	402 KB
TiSmelting_database.cst	01-07-2021 10:20	CST File	151 KB

The 'BOF_database.cst' file is selected. The 'Open' button is highlighted with a red box. A 'Load CST Database' dialog is open, showing the file path 'lib\Database.cst'. The 'LOAD' button is highlighted with a red box. The 'OK' button is also highlighted with a red box.

In the browse window, select a database file (*.cst) and click open

Click to change/load the current database file

⚠ Click OK to save the change in the program

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 - Using Equations in the modules
 - Transferring material to the next step
 - Changing global and local units
 - Manage Splitter and Equilib Process IDs
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Step 2: Build the process flowsheet

Enter the number of steps (= number of Times the flowsheet is repeated during run)

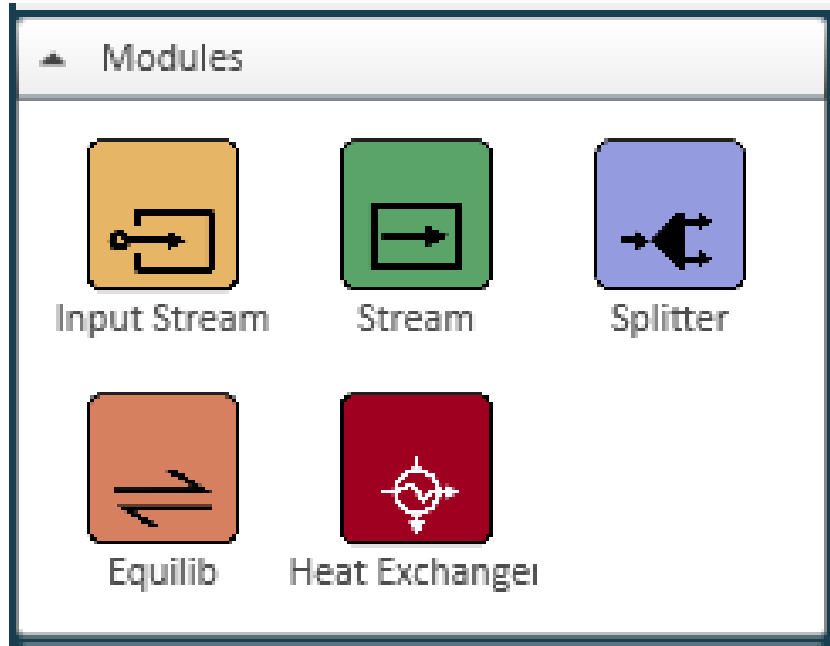
The process flowsheet is built in the diagram workspace by adding flowsheet objects from the modules panel and connecting them with arrows to indicate material flow

The flowsheet modules include:

- 2 types of Streams (Input stream and Stream)
- 3 types of Unit Operations (Splitter, Equilib and Heat Exchanger)

Version: 2.1.8909

Modules Panel



Choose one of the modules based on the intent:

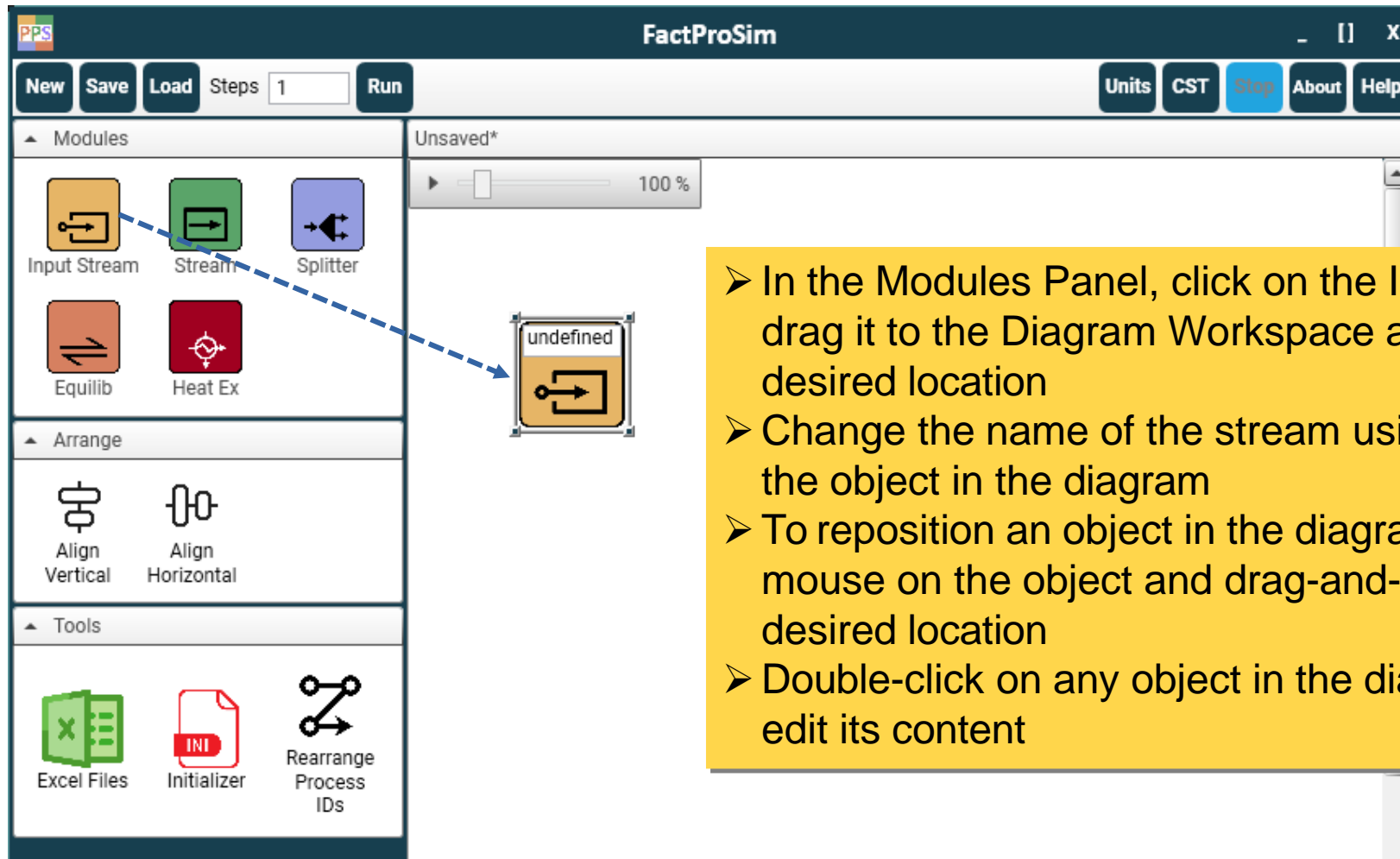
- **Input Stream:** define starting materials for the simulation (mass, temperature, composition and phase selection)
- **Stream:** convey the equilibrated material information between units (phase selection)
- **Splitter:** split the incoming stream into two or more streams according to a specified split fraction or amount
- **Equilib:** perform equilibrium calculations with given reactant streams, selected products and final conditions (temperature, enthalpy, pressure)
- **Heat Exchanger:** perform heat exchange between two streams (no other reaction only heat exchange), with given conditions (Temperature or Enthalpy)

How to use: drag and drop one of the modules from the Modules Panel into the Diagram (flowsheet) Workspace

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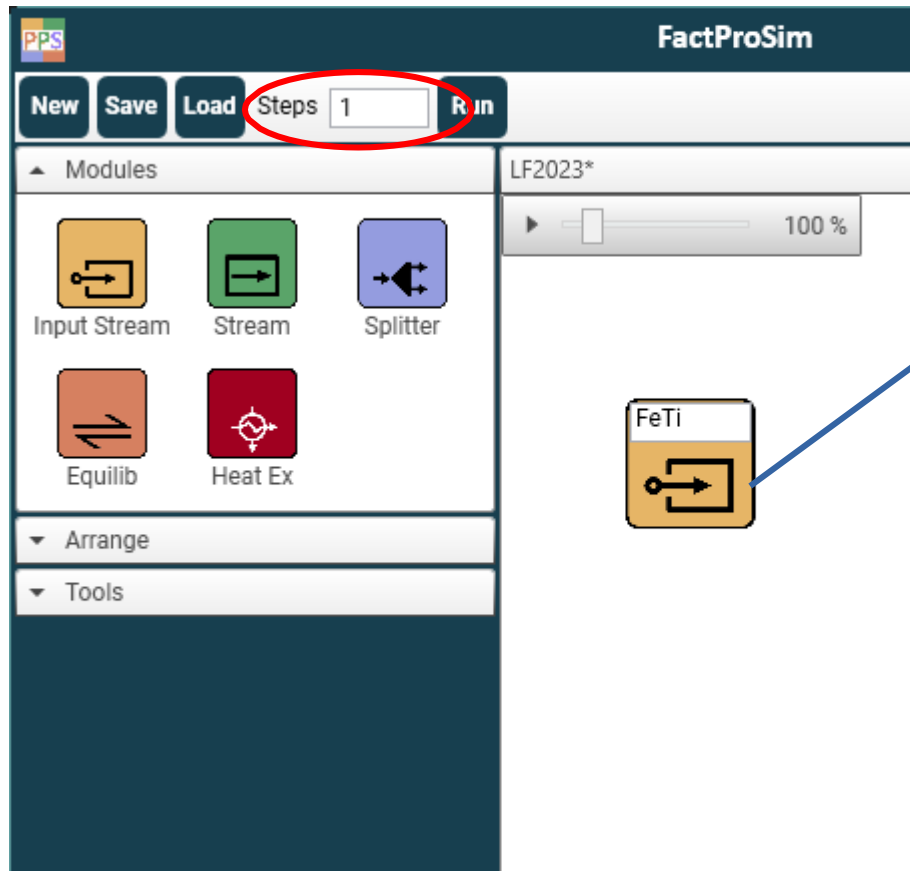
Adding an Input Stream in the diagram



- In the Modules Panel, click on the Input Stream icon, drag it to the Diagram Workspace and drop it at the desired location
- Change the name of the stream using the text box on the object in the diagram
- To reposition an object in the diagram, position the mouse on the object and drag-and-drop it to the desired location
- Double-click on any object in the diagram to view and edit its content

Input Stream Module – Manual entry, 1 step

Change the units for this specific module ([see Global and local Units](#))



Local Units Description: Excel Link Equation

Name FeTi

Temperature (C) 25

Amount (g) 0

Pressure (atm) 1

Components ADD

Mass Percent	Species
0.4	N
0.2	C
0.006	S
0	Mg
4.5	Al
0.21	Si
0.01	P

Total%: 100

Change the name of the stream (same function from the module textbox)

Enter the Temperature, Amount and Pressure

- List all the components (chemical formula only, ex: Fe, CaO) and their composition (in percentage), 1 component per line
- Press the button 'Add' to add a new component (new line)
- The total content is indicated at the bottom

Input Stream Module – Manual entry, 1 step

The screenshot displays the FactProSim interface. The 'Steps' field is highlighted with a red circle and contains the value '1'. The 'Input Stream' module is selected, and its configuration panel is shown on the right. The 'Components' table is as follows:

Mass Percent	Species
Bal.	Fe
0.4	N
0.2	C
0	Mg
4.5	Al

The 'Total%: 100' field is also highlighted with a red box. A callout box explains the 'Bal.' keyword: "The 'Bal.' keyword will automatically assign the remaining mass/mole to the corresponding element, and make the sum of the composition equal to '100'".

Input Stream Module – Phase selection

The screenshot shows the 'Input Stream' dialog box. On the left, there are input fields for Name (FeTi), Temperature (25 C), Amount (0 g), and Pressure (1 atm). Below these are 'Excel Link' and 'Equation' checkboxes, and a 'Components' section with an 'ADD' button and a table of mass percent and species. The main area is divided into three categories: 'Gas Phase Species', 'Solution Phases', and 'Pure Solids'. The 'Pure Solids' category is selected, and 'C_Graphite(s)' and 'Mg_solid(s)' are checked. A red box highlights the species and phase lists. At the bottom, there are 'OK' and 'Schedule' buttons.

Mass Percent	Species
0.4	N
0.2	C
0.006	S
0	Mg
4.5	Al
0.21	Si
0.01	P

Gas Phase Species	Solution Phases	Pure Solids
<input type="checkbox"/> C	<input type="checkbox"/> BCC_A2	<input checked="" type="checkbox"/> C_Graphite(s)
<input type="checkbox"/> C2	<input type="checkbox"/> Slag-liq	<input checked="" type="checkbox"/> Mg_solid(s)
<input type="checkbox"/> C3		
<input type="checkbox"/> C4		
<input type="checkbox"/> C5		
<input type="checkbox"/> N		
<input type="checkbox"/> N2		
<input type="checkbox"/> N3		
<input type="checkbox"/> CN		
<input type="checkbox"/> C2N		
<input type="checkbox"/> CNN(g)		
<input type="checkbox"/> CNN(g2)		
<input type="checkbox"/> (CN)2		
<input type="checkbox"/> C4N2		
<input type="checkbox"/> O		
<input type="checkbox"/> O2		
<input type="checkbox"/> O3		
<input type="checkbox"/> CO		

Phase Selection:

- The available phases are automatically populated from the selected database file, based on the entered components. They are organised into 3 categories: gas species, solution phases and pure solids
- Use the checkbox in front of the species or phase to select it. Multiple phases and species can be selected throughout more than 1 category
- ⚠ at least one species, solution or pure solids must be selected
- Use the 'All' checkbox to select all species or phases in a given category

Input Stream Module – Manual entry, >1 step

When more than 1 step is defined in the Toolbar, different values can be used at each step
💡 A schedule is needed to enter these values
The Schedule button becomes available at the bottom of the module

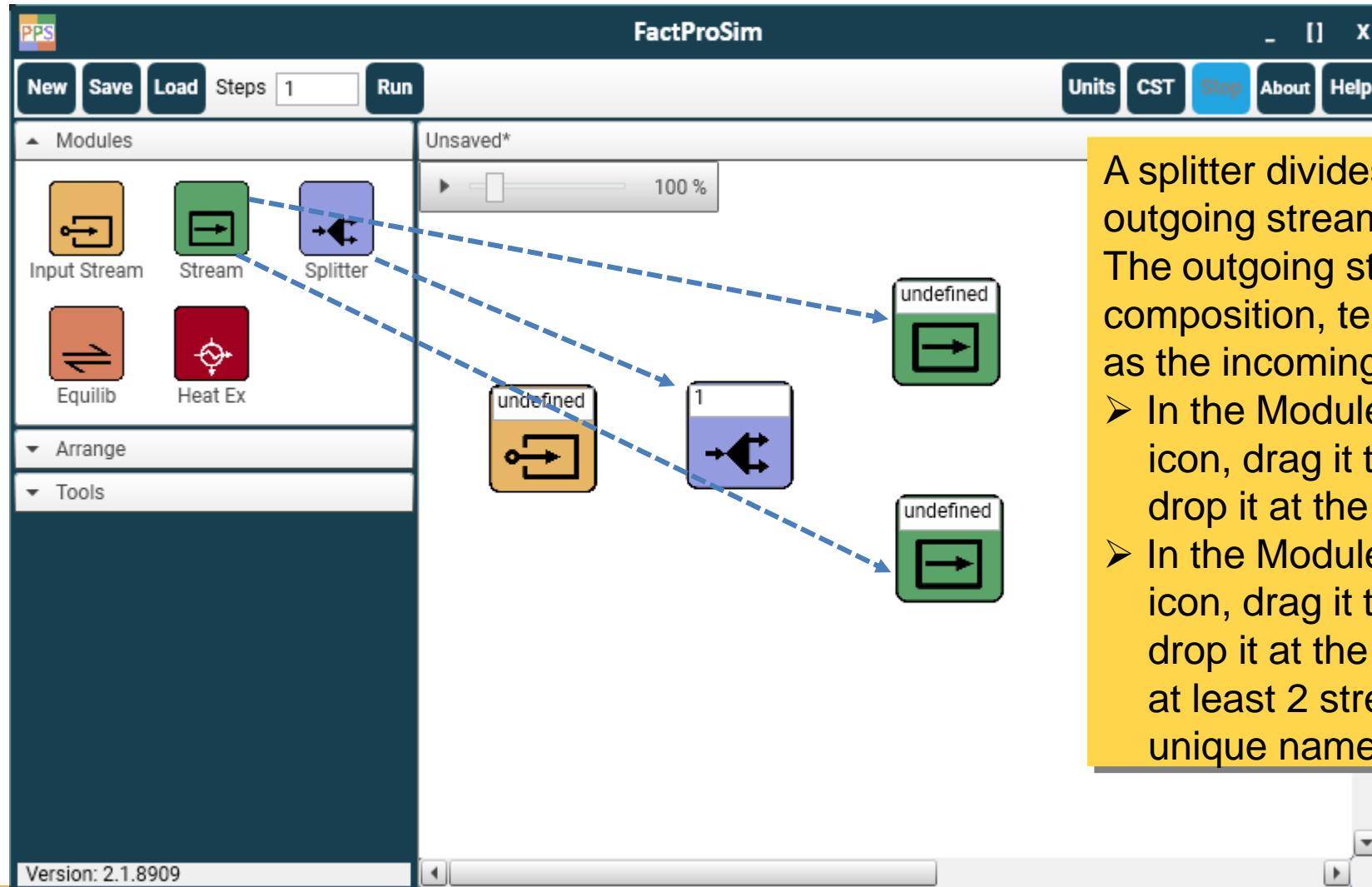
Enter the desired values for each time step in the table
⚠ Each entry must be filled!

Time	Temperature	Amount	Pressure
1	1200	20	1
2	1200	20	1
3	1200	20	1
4	1200	20	1
5	1200	20	1
6	1200	20	1
7	1200	20	1
8	1200	20	1
9	1200	20	1
10	1200	20	1

Description of the program

- Overview of the main window and commands in the Toolbar
- Step 1: Create and load a database file
- Step 2: Build the Process Flowsheet
 - Modules Panel
 - Input Stream module
 - **Splitter module**
 - Equilib module
 - Heat Exchanger module
 - Using Excel Links in the modules
 - Using Equations in the modules
 - Transferring material to the next step
 - Changing global and local units
 - Manage Splitter and Equilib Process IDs
 - Align the process modules in the flowsheet
 - Save and load an existing flowsheet
- Step 3: Check the modules – The Initializer
- Step 4: Run the process flowsheet
- Step 5: View the Results (Output Excel File)

Adding a Splitter and streams in the diagram



A splitter divides an incoming stream into several outgoing streams with defined split conditions. The outgoing streams have the same composition, temperature and phase selection as the incoming stream

- In the Modules Panel, click on the Splitter icon, drag it to the Diagram Workspace and drop it at the desired location
- In the Modules Panel, click on the Stream icon, drag it to the Diagram Workspace and drop it at the desired location. Repeat to have at least 2 streams in the diagram. Enter a unique name for each stream

Connecting modules with arrows (Material flow)

FactProSim

New Save Load Steps 1 Run

Modules

Input Stream Stream Splitter

Equilib Heat Ex

Arrange

Tools

Unsaved*

100 %

Connectors

Input

1

Drag and Drop the line to one of the other module

Input

1

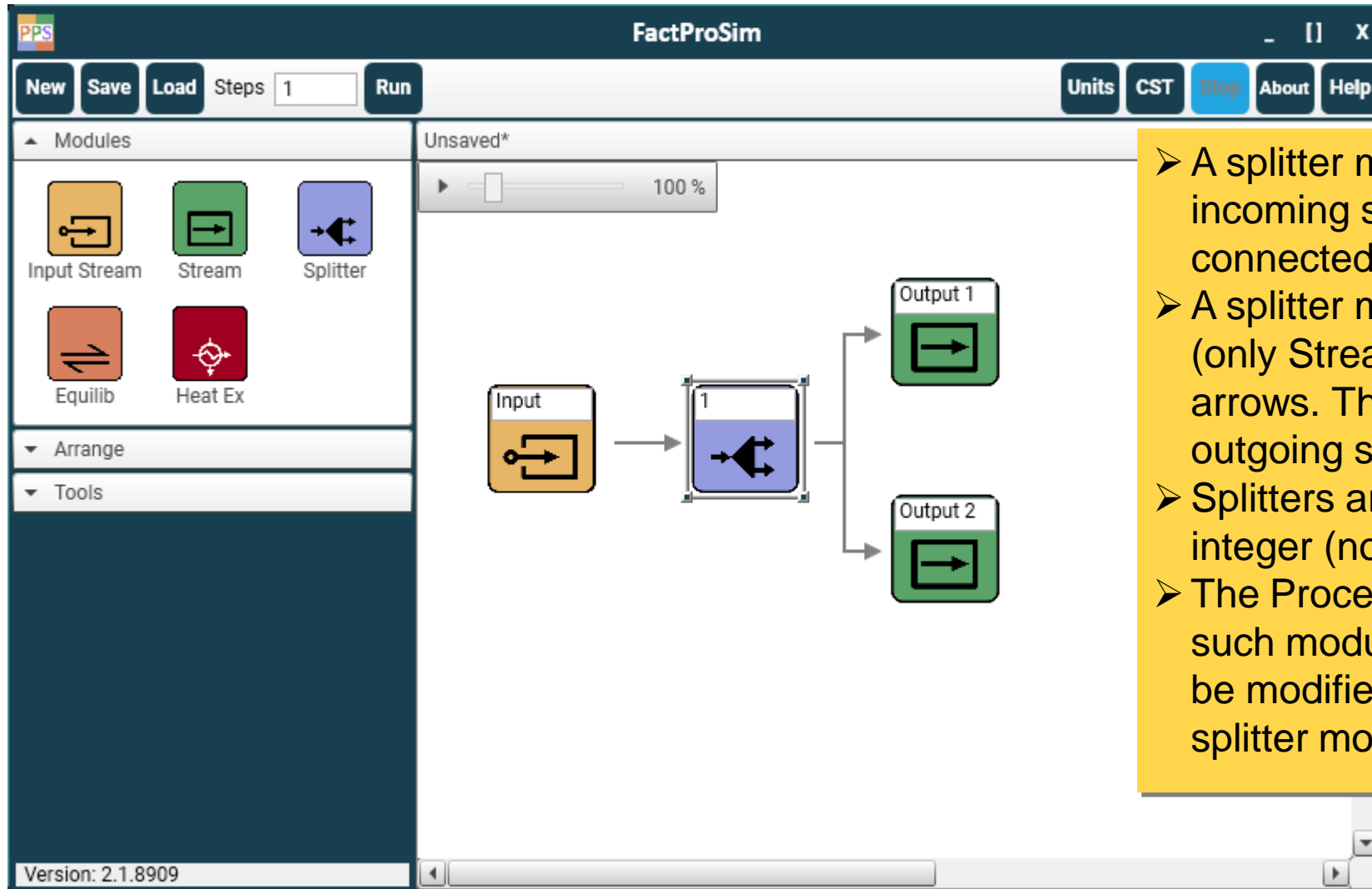
Output

Output 2

- In the Diagram, place the mouse cursor on the object (module) from which the material is flowing
- Click on one of the 4 connectors located at each side of the object and drag the line toward the object to be connected to
- Release the cursor (drop the line) in or near one of the 4 connectors of the object to be connected to

Version: 2.1.8909

Adding a Splitter and streams in the diagram



- A splitter must have one **(and only one)** incoming stream (Input Stream or Stream) connected with an inbound arrow
- A splitter must have at least 1 outgoing stream (only Stream objects) connected with outbound arrows. There is no limit in the number of outgoing streams
- Splitters are identified by a unique Process ID integer (not a text label like streams)
- The Process ID is automatically assigned when such module is inserted in the Diagram. It can be modified by the user from the label on the splitter module

Splitter Module – Manual entry, 1 step

FactProSim

Load Steps 1 Run

Summary

Unsaved* 100 %

Stream Splitter Heat Exchanger

Input 1

Assign one or more outgoing streams as balance (Bal.) by selecting the checkbox

Splitter

Description: No Description

Percent Amount (kg)

Bal?	Value	Outgoing Stream	Excel Link	Equation
<input type="checkbox"/>	80	Output 1	<input type="checkbox"/>	<input type="checkbox"/>
<input checked="" type="checkbox"/>	Bal.	Output 2	<input type="checkbox"/>	<input type="checkbox"/>

List of all outgoing streams

Select split percentage or absolute amount

- The term Bal. indicates that the stream contains the remaining percentage or amount of incoming stream. If more than one outgoing stream is set as Bal., the remaining percentage or amount of incoming stream is shared equally among them
- The splitter is set initially with all outgoing streams as Bal. (incoming stream amount is equally shared among all outgoing streams)
- To ensure mass balance conservation, at least one outgoing stream must be assigned as balance

Splitter Module – Manual entry, >1 step

The screenshot displays the FactProSim software interface. On the left, a toolbar contains buttons for 'New', 'Save', 'Load', 'Steps' (set to 10), and 'Run'. Below the toolbar is a 'Modules' panel with icons for 'Input Stream', 'Stream', 'Splitter', 'Equilib', and 'Heat Exchanger'. The main window shows the 'Splitter' configuration dialog. It includes a 'Description' field (set to 'No Description'), an 'Incoming Stream' section, and an 'Input' section with 'Process ID' set to 1. The 'Incoming Stream' section has radio buttons for 'Percent' (selected) and 'Amount (kg)'. The 'Input' section has a table with columns 'Bal?', 'Value', 'Outgoing Stream', 'Excel Link', and 'Equation'. Two rows are visible: 'Output 1' with 'Bal?' unchecked and 'Output 2' with 'Bal?' checked. Below the configuration are 'OK' and 'Schedule' buttons. To the right, a 'Splitter Schedule' window shows a table with columns 'Time', 'Output 1', and 'Output 2'. The table contains 10 rows, with 'Output 1' values of 80 and 'Output 2' values of 'Bal.' for all time steps. A yellow callout box on the left explains that when more than 1 step is defined, a schedule is needed. A yellow callout box on the right explains that 'Bal.' values are not editable and that each entry must be filled or the program will assume 'Bal.'.

When more than 1 step is defined in the toolbar, different values can be used at each step
💡 A schedule is needed to enter these values
The Schedule button becomes available at the bottom of the module

Time	Output 1	Output 2
1	80	Bal.
2	80	Bal.
3	80	Bal.
4	80	Bal.
5	80	Bal.
6	80	Bal.
7	80	Bal.
8	80	Bal.
9	80	Bal.
10	80	Bal.

Enter the desired values for each time step in the table The column(s) of the outgoing stream(s) checked as Bal. are not editable
⚠️ Each entry must be filled or the program will assume Bal.

Splitter Module – Outgoing streams

FactProSim

New Save Load Steps 1 Run

Modules

- Input Stream
- Stream
- Splitter
- Equilib
- Heat Ex

Arrange

Tools

Unsaved* 100%

Input

1

Output 1

Output 2

Stream

Description: No Description

Name: Output 1

Units for Printing

Gas Phase Species	All	Solution Phases	All	Pure Solids	All
<input checked="" type="checkbox"/> Ca	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/> Slag-liq	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/> Ca_Solid_Alpha(s)	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/> Ca2	<input checked="" type="checkbox"/>			<input checked="" type="checkbox"/> CaO_Lime(s)	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/> O	<input checked="" type="checkbox"/>			<input checked="" type="checkbox"/> Si_solid(s)	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/> O2	<input checked="" type="checkbox"/>			<input checked="" type="checkbox"/> CaSi2_hR18-R3m(s)	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/> O3	<input checked="" type="checkbox"/>			<input checked="" type="checkbox"/> Ca2Si_oP12-Pnma(s)	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/> CaO	<input checked="" type="checkbox"/>			<input checked="" type="checkbox"/> SiO2_Quartz(l)(s)	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/> Si	<input checked="" type="checkbox"/>			<input checked="" type="checkbox"/> SiO2_Tridymite(h)(s4)	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/> Si2	<input checked="" type="checkbox"/>			<input checked="" type="checkbox"/> SiO2_Cristobalite(h)(s6)	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/> Si3	<input checked="" type="checkbox"/>			<input checked="" type="checkbox"/> CaSiO3_Wollastonite(s)	<input checked="" type="checkbox"/>
<input checked="" type="checkbox"/> SiO	<input checked="" type="checkbox"/>			<input checked="" type="checkbox"/> Ca2SiO4_Gamma(olivine(s))	<input checked="" type="checkbox"/>

Total Selection: 14 Total Selection: 1 Total Selection: 15

OK

Version: 2.1.8909

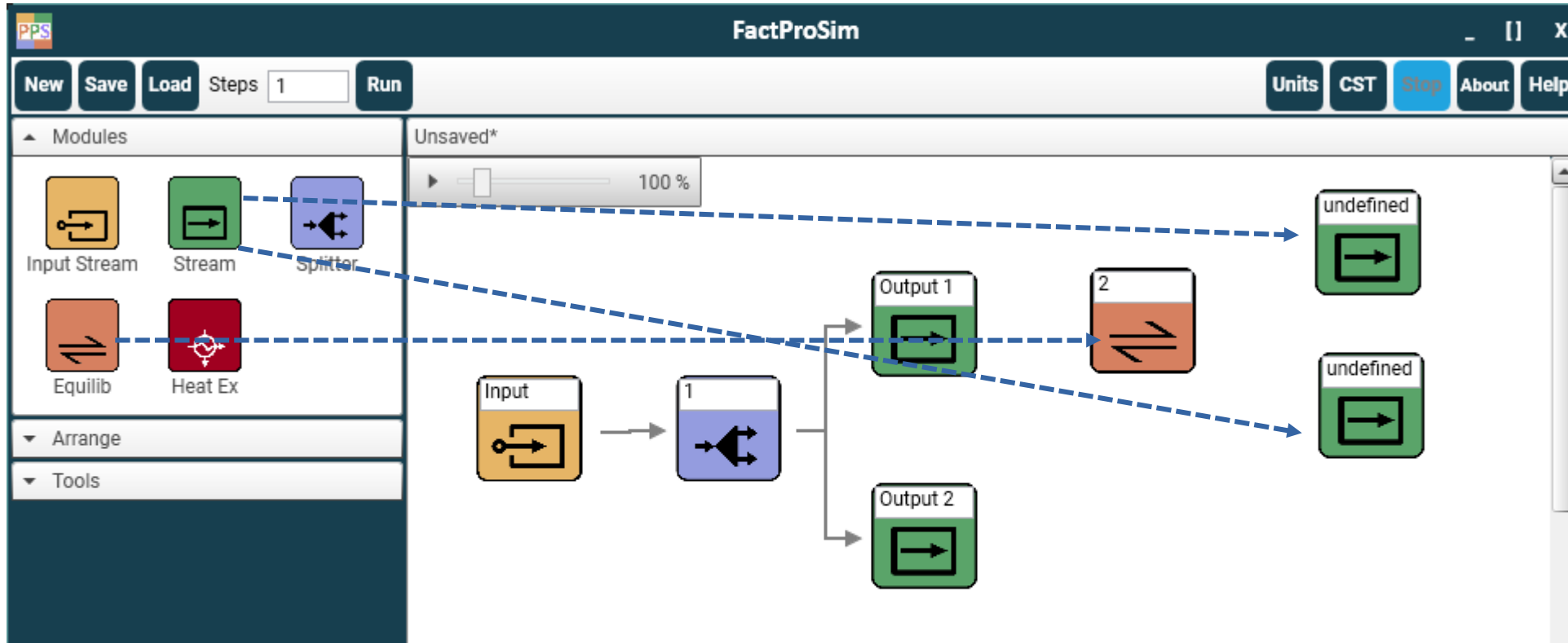
➤ There is nothing to edit in the outgoing streams connected to a splitter

➤ The phase selection, temperature and composition are defined by the incoming stream and cannot be modified

Description of the program

- Overview of the main window and commands in the Toolbar
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 - **Equilib module**
 - Heat Exchanger module
 - Using Excel Links in the modules
 - Using Equations in the modules
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 - Changing global and local units
 - Manage Splitter and Equilib Process IDs
 - Align the process modules in the flowsheet
 - Save and load an existing flowsheet
- Step 3: Check the modules – The Initializer
- Step 4: Run the process flowsheet
- Step 5: View the Results (Output Excel File)

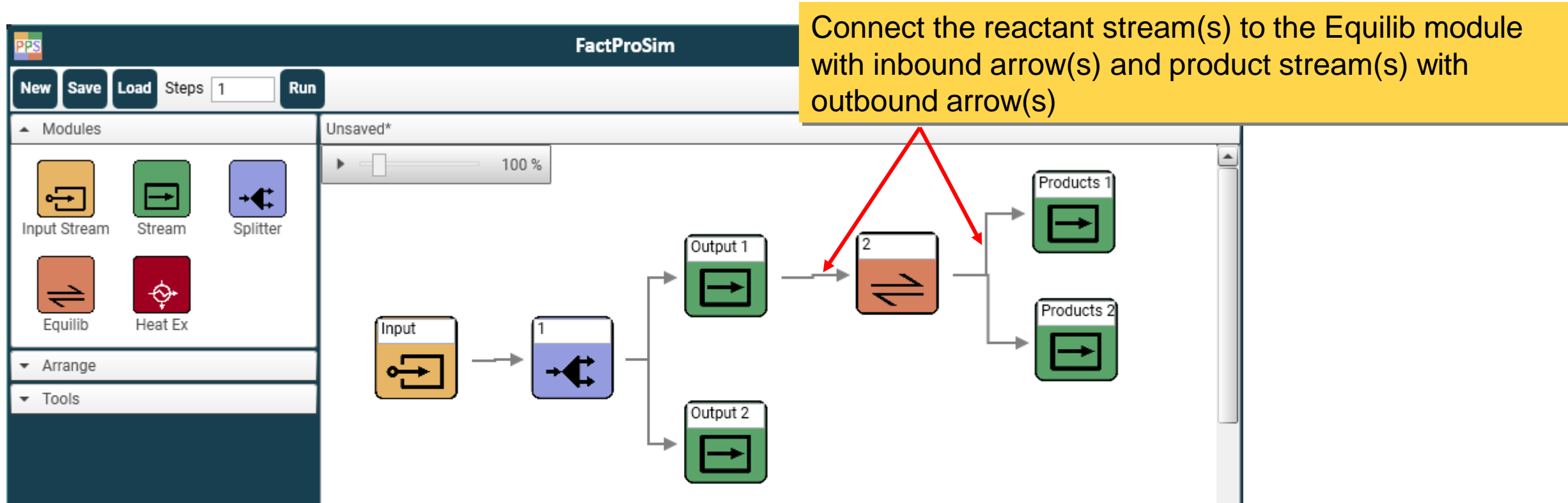
Add Equilib module and reactant streams in the diagram



An Equilib module allows to perform an equilibrium reaction given the connected reactant stream(s) and equilibrium conditions set in the module

- In the Modules Panel, click on the Equilib icon, drag it to the Diagram Workspace and drop it at the desired location
- Depending on the desired reaction, drag-and-drop additional Input Stream(s) (reactant) and Streams (reaction products). Enter a unique name for each stream

Add Equilib module and reactant streams in the diagram



- An Equilib must have at least one incoming stream (Input Stream or Stream) connected with an inbound arrow. There is no limit in the number of incoming streams
- There are no restrictions in the number of outgoing streams (only Stream objects)
- Equilib is identified by a unique Process ID integer (not a text label like streams)
- The Process ID is automatically assigned when such module is inserted in the Diagram. It can be modified by the user from the label on the Equilib module

Equilib Module – Manual entry, 1 step

Change the units for this specific module (see [Global and local Units](#))

Local Units

Description: No Description

Excel Link Equation Gas Phase Species

Temperature (C) 1500

Enthalpy (J)

Pressure (atm) 1

Process ID 2

Incoming Streams

Output 1

Outgoing Streams

Products 1

Products 2

Skip if No Reactants

Total Selection: 0

Total Selection: 0

Total Selection: 0

CaO_Lime(s)

CaSiO3_Wollastonite(s)

Ca2SiO4_Gamma(olivine(s))

Ca2SiO4_Alpha-prime(s2)

Define the final conditions of the equilibrium calculation

⚠ only 2 of the 3 fields must be filled, one field must be empty:

- Provide the temperature and pressure for isothermal calculation (enthalpy field empty)
- Provide the enthalpy and pressure for adiabatic calculations (temperature field empty)

Summary of incoming and outgoing streams and Process ID

Choose this option when you want to move the reaction forward even when incoming streams don't contain anything

⚠ This is dangerous and should be done fully realizing the effect of it

Equilib Module – Manual entry, 1 step

Phase Selection:

- The available phases are automatically populated from the selected database file, based on the incoming streams. They are organised into 3 categories: gas species, solution phases and pure solids
- Use the checkbox in front of the species or phase to select it. Multiple phases and species can be selected throughout more than 1 category
- ⚠ at least one species, solution or pure solids must be selected
- Use the 'All' checkbox to select all species or phases in a given category

The screenshot shows the 'Equilib' software window with a 'Description' field containing 'No Description'. Below this, there are three columns of phase selection options, each with an 'All' checkbox and a list of individual species/phase checkboxes. The 'Gas Phase Species' column has 14 items, all checked. The 'Solution Phases' column has 5 items, with 'Slag-liq' checked. The 'Pure Solids' column has 11 items, with 'CaO_Lime(s)' checked. At the bottom of each column, the 'Total Selection' is displayed: 14 for Gas Phase Species, 1 for Solution Phases, and 1 for Pure Solids. There are 'OK' and 'Schedule' buttons at the bottom of the window.

Equation	Gas Phase Species	Solution Phases	Pure Solids
<input type="checkbox"/>	<input checked="" type="checkbox"/> O	<input type="checkbox"/> BCC_A2	<input type="checkbox"/> Mg_solid(s)
<input type="checkbox"/>	<input checked="" type="checkbox"/> O2	<input checked="" type="checkbox"/> Slag-liq	<input type="checkbox"/> Si_solid(s)
<input type="checkbox"/>	<input checked="" type="checkbox"/> O3	<input type="checkbox"/> Monoxide#1	<input type="checkbox"/> Ca_Solid_Alpha(s)
<input type="checkbox"/>	<input checked="" type="checkbox"/> Mg	<input type="checkbox"/> Monoxide#2	<input type="checkbox"/> CaSi2_hR18-R3m(s)
	<input checked="" type="checkbox"/> Mg2	<input type="checkbox"/> Fe-liq	<input type="checkbox"/> Ca2Si_oP12-Pnma(s)
	<input checked="" type="checkbox"/> MgO		<input type="checkbox"/> MgO_periclase(s)
	<input checked="" type="checkbox"/> Si		<input type="checkbox"/> SiO2_Quartz(l)(s)
	<input checked="" type="checkbox"/> Si2		<input type="checkbox"/> SiO2_Tridymite(h)(s4)
	<input checked="" type="checkbox"/> Si3		<input type="checkbox"/> SiO2_Cristobalite(h)(s6)
	<input checked="" type="checkbox"/> SiO		<input checked="" type="checkbox"/> CaO_Lime(s)
	<input checked="" type="checkbox"/> SiO2		<input type="checkbox"/> CaSiO3_Wollastonite(s)
	<input checked="" type="checkbox"/> Ca		<input type="checkbox"/> Ca2SiO4_Gamma(olivine(s)
	<input checked="" type="checkbox"/> Ca2		<input type="checkbox"/> Ca2SiO4_Alpha-prime(s2)

Total Selection: 14 Total Selection: 1 Total Selection: 1

Equilib Module – Manual entry, >1 step

The screenshot shows the Equilib module interface. In the top toolbar, the 'Steps' field is set to 10. The 'Equilib' button is highlighted with a red box. The 'Schedule' button is also highlighted with a red box. The 'Equilib Schedule' table is shown on the right, with columns for Time, Temperature, Enthalpy, and Pressure. The table contains 10 rows, all with a Temperature of 1500 and Pressure of 1. The 'Equilib' module settings are visible in the background, including 'Local Units' and 'Gas Phase Species'.

When more than 1 step is defined in the toolbar, different values can be used at each step
💡 A schedule is needed to enter these values
The Schedule button becomes available at the bottom of the module

Enter the desired values for each time step in the table
⚠️ Specify only 2 conditions at each line, one condition must be empty

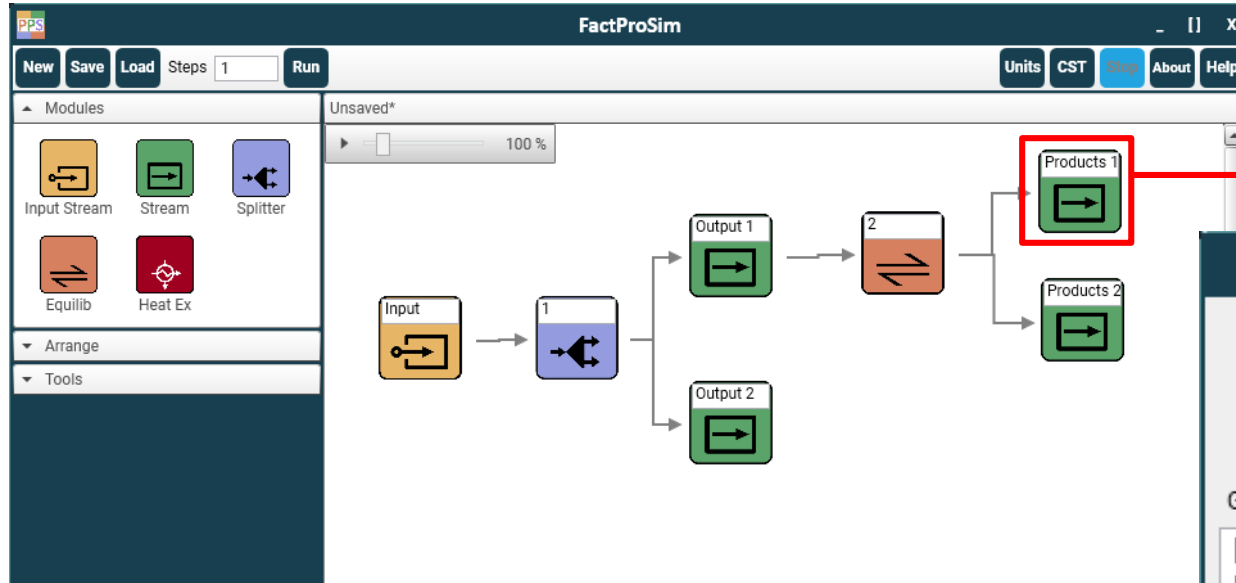
Time	Temperature	Enthalpy	Pressure
1	1500		1
2	1500		1
3	1500		1
4	1500		1
5	1500		1
6	1500		1
7	1500		1
8	1500		1
9	1500		1
10	1500		1

Equilib Module – Outgoing streams (reaction products)

The screenshot shows the FactProSim software interface. The title bar reads "FactProSim". The menu bar includes "New", "Save", "Load", "Steps" (with a value of 1), "Run", "Units", "CST", "Stop", "About", and "Help". The main workspace displays a process flow diagram. On the left, a vertical toolbar contains icons for "Input Stream" (orange), "Equilib" (red), and "Arrange" (blue). The "Equilib" module is represented by a red box with a double-headed arrow. Two outgoing streams, labeled "Products 1" and "Products 2", are shown as green boxes with right-pointing arrows. These two product boxes are circled in red. A yellow callout box is overlaid on the diagram, containing three bullet points. The status bar at the bottom left shows "Version: 2.1.8909".

- The outgoing streams do not affect the Equilib calculations
- The phase selection of the reaction products is defined exclusively in the Equilib module, and is not affected by the presence and phase selection in the outgoing streams connected to the Equilib module
- The function of the outgoing streams is only to transfer some or all the equilibrated material from the Equilib module to another unit

Equilib Module – Outgoing streams (reaction products)



Change the local units when printing the content of this stream in its Excel worksheet

Description: No Description

Name: Products 1

Units for Printing

Gas Phase Species	Solution Phases	Pure Solids
<input type="checkbox"/> O	<input type="checkbox"/> Slag-liq	<input type="checkbox"/> CaO_Lime(s)
<input type="checkbox"/> O2		
<input type="checkbox"/> O3		
<input type="checkbox"/> Mg		
<input type="checkbox"/> Mg2		
<input type="checkbox"/> MgO		
<input type="checkbox"/> Si		
<input type="checkbox"/> Si2		
<input type="checkbox"/> Si3		
<input type="checkbox"/> SiO		

Total Selection: 0 Total Selection: 0 Total Selection: 0

OK

- The outgoing streams contain the list of phases that have been selected in the upstream Equilib
- Use the checkbox in front of the species or phase to select it. Multiple phases and species can be selected throughout more than 1 category
 - ⚠ at least 1 species, solution or pure solid must be selected
 - Use the 'All' checkbox to select all species or phases in a given category

Equilib Module – Outgoing streams (reaction products)

Units CST Stop About Help

Stream

Description: No Description

Name Products 1

Gas Phase Species All

- O
- O2
- O3
- Mg
- Mg2
- MgO

Stream

Description: No Description

Name Products 2

Units for Printing

Gas Phase Species All Solution Phases All Pure Solids All

- O
- O2
- O3
- Mg
- Mg2
- MgO
- Si
- Si2
- Si3
- SiO

Slag-liq

CaO_Lime(s)

Total Selection: 0

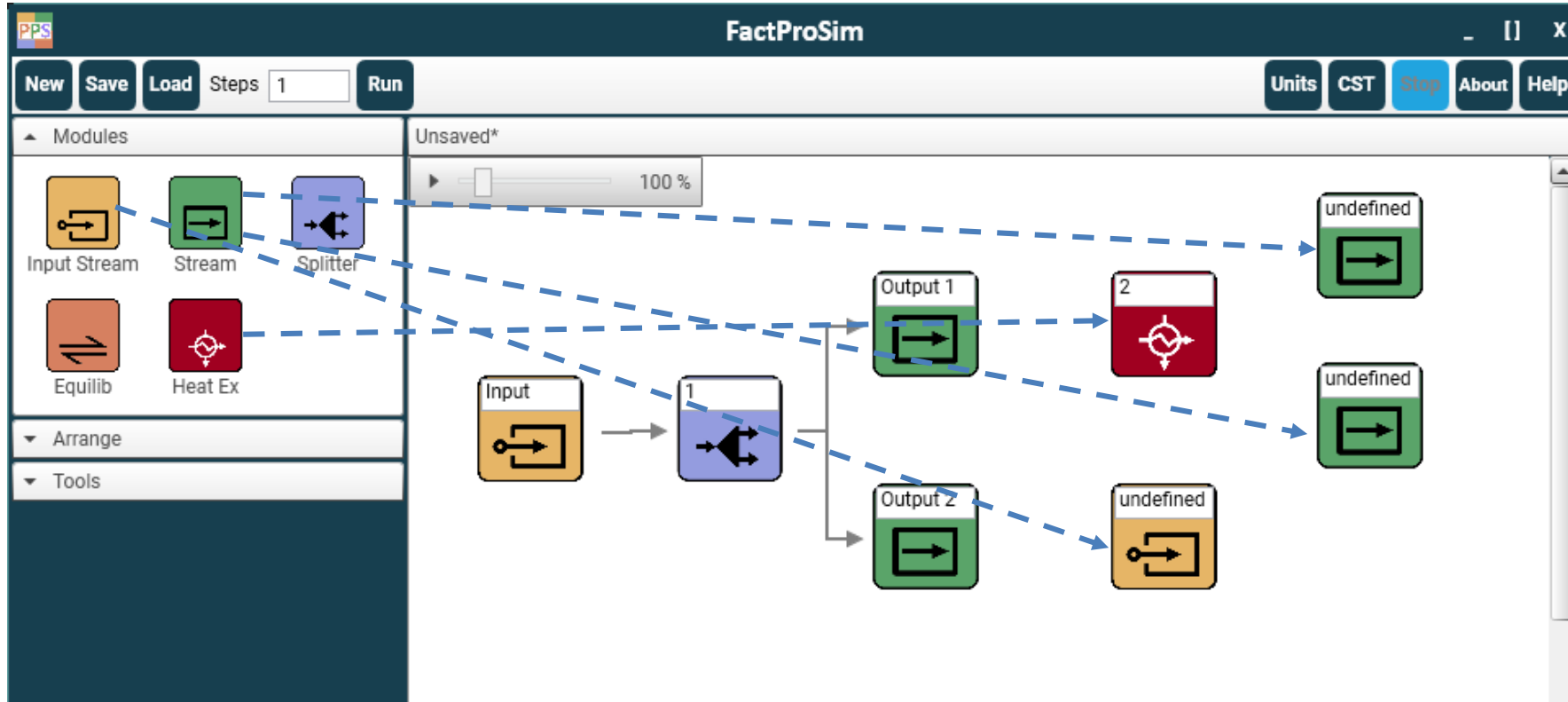
These phases cannot be selected in this stream since they are already selected in the other connected stream

- The outgoing streams connected to the same Equilib are linked: once a species, solution phase or pure solid is selected in one outgoing stream, the same species, solution phase or pure solid cannot be selected in another outgoing stream
- It is not necessary to match the entire phase selection made in the upstream Equilib. However, the unselected phases cannot be transferred to another module and will not be printed in the output Excel sheet

Description of the program

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 - Equilib module
 - **Heat Exchanger module**
 - Using Excel Links in the modules
 - Using Equations in the modules
 - Transferring material to the next step
 - Changing global and local units
 - Manage Splitter and Equilib Process IDs
 - Align the process modules in the flowsheet
 - Save and load an existing flowsheet
- Step 3: Check the modules – The Initializer
- Step 4: Run the process flowsheet
- Step 5: View the Results (Output Excel File)

Add Heat Exchanger and reactant streams in the diagram

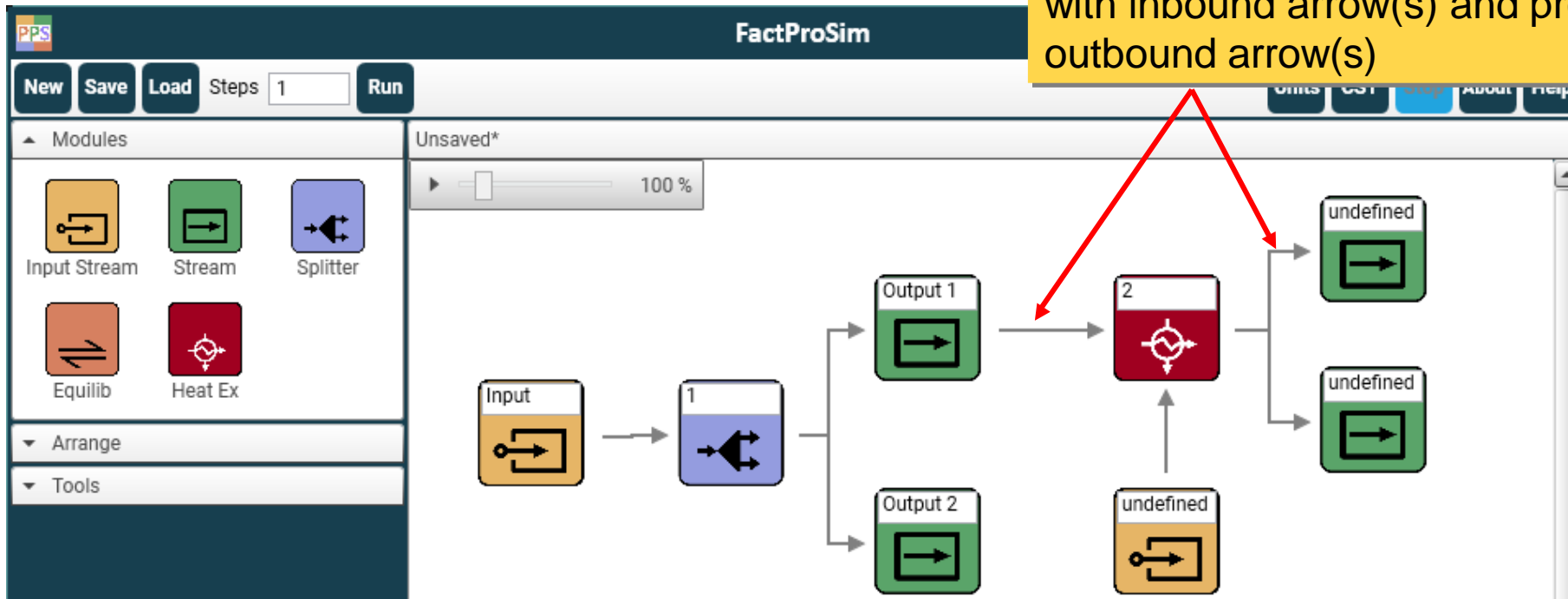


A Heat Exchanger allows to perform heat exchange between two reactant stream(s) and conditions set inside the module

- In the Modules Panel, click on the Heat Exchanger icon, drag it to the Diagram Workspace and drop it at the desired location
- Depending on the desired reaction, drag-and-drop additional Input Stream(s) (reactant) and Streams (reaction products). Enter a unique name for each stream

Add Heat Exchanger and reactant streams in the diagram

Connect the reactant stream(s) to the Heat Exchanger with inbound arrow(s) and product stream(s) with outbound arrow(s)



- A Heat Exchanger must have two incoming stream (Input Stream or Stream) connected with an inbound arrow. Only two streams are allowed for inbound material flow
- There are no restrictions in the number of outgoing streams (only Stream objects)
- Heat Exchanger is identified by a unique Process ID integer (not a text label like streams)
- The Process ID is automatically assigned when such module is inserted in the Diagram. It can be modified by the user from the label on the Heat Exchanger module

Heat Exchanger Module – Manual entry, 1 step

Heat Exchanger

Description: No Description

Incoming Streams Outgoing Streams Excel Link Equation

Temperature difference (C)

Temperature Change (C)

Enthalpy Change (J)

Input 2 Output 1

Input 2 Output 1

Input 2

Output 1

Products 1

Products 2

Products 1

Products 2

Skip if No Reactants

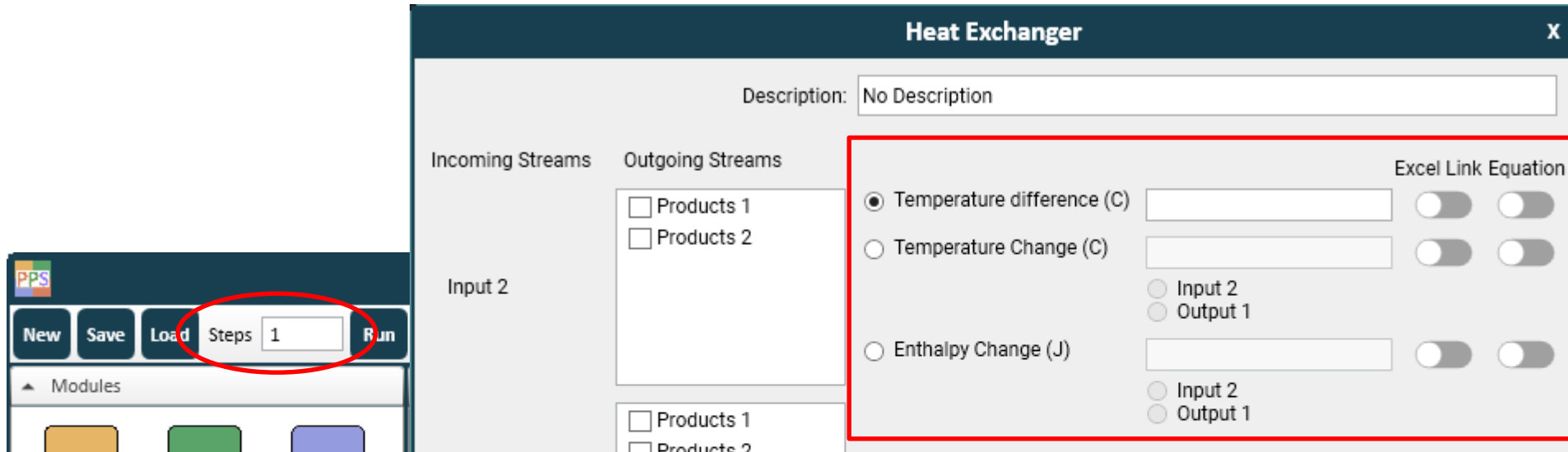
OK

Summary of incoming and outgoing streams

Choose this option when you want to move the reaction forward even when incoming streams don't contain anything

⚠ This is dangerous and should be done fully realizing the effect of it

Heat Exchanger Module – Manual entry, 1 step



Define the final conditions of the equilibrium calculation

You can select one of the 3 conditions:

- Final Temperature Difference between streams, it will raise the temperature of the colder stream and lower the temperature of the hotter stream to achieve the temperature difference, **only +value accepted here**
- Temperature change of one stream, after selecting this option, you have to select the stream whose temperature you want to change, +value means increase, -value means decrease
- Enthalpy change of one stream, after selecting this option, you have to select the stream whose enthalpy you want to change, +value means increase, -value means decrease

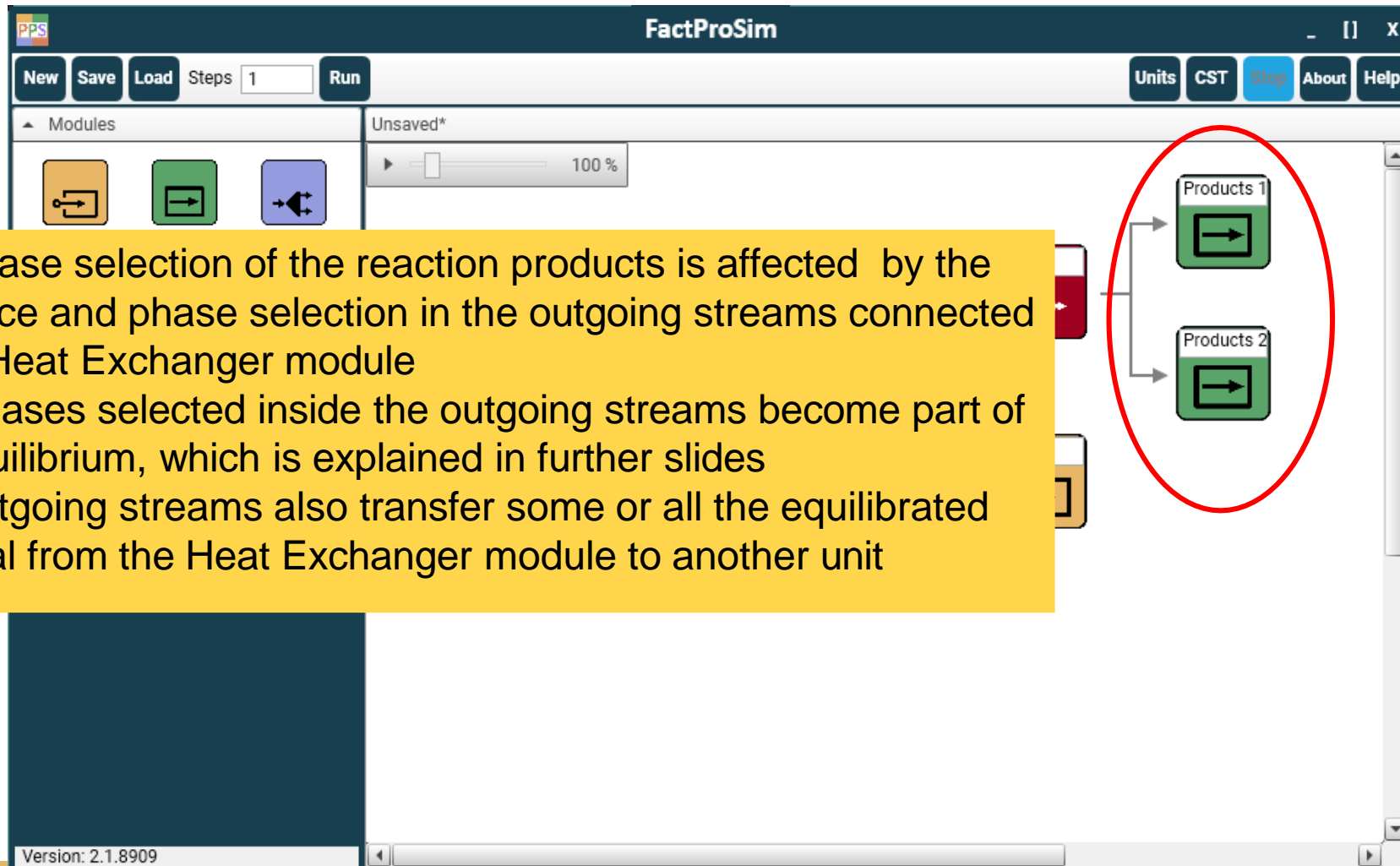
Heat Exchanger Module – Manual entry, >1 step

The screenshot displays the FactProSim software interface. On the left, a toolbar contains buttons for 'New', 'Save', 'Load', 'Steps' (set to 10), and 'Run'. Below the toolbar is a 'Modules' panel with icons for 'Input Stream', 'Stream', 'Splitter', 'Equilib', and 'Heat Exchanger'. The main window is titled 'Heat Exchanger' and contains a 'Description' field with 'No Description'. It features 'Incoming Streams' and 'Outgoing Streams' sections. Under 'Incoming Streams', 'Products 2' is selected. Under 'Outgoing Streams', 'Products 1' is selected. The 'Temperature difference (C)' option is selected, with 'Check Schedule' and 'Excel Link Equation' options. The 'Schedule' button is highlighted with a red box. A red arrow points from the 'Schedule' button to the 'Heat Exchanger Schedule' table on the right. The table has columns for 'Time', 'Temperature Difference', 'Temperature Change', and 'Enthalpy Change'. The 'Temperature Difference' column contains the value 10 for all 10 time steps. A yellow box with the text 'Enter the desired values for each time step in the table' is overlaid on the table. An 'OK' button is located below the table.

When more than 1 step is defined in the toolbar, different values can be used at each step
💡 A schedule is needed to enter these values
The Schedule button becomes available at the bottom of the module

Time	Temperature Difference	Temperature Change	Enthalpy Change
1	10		
2	10		
3	10		
4	10		
5	10		
6	10		
7	10		
8	10		
9	10		
10	10		

Heat Exchanger– Outgoing streams (reaction products)



- The phase selection of the reaction products is affected by the presence and phase selection in the outgoing streams connected to the Heat Exchanger module
- The Phases selected inside the outgoing streams become part of the Equilibrium, which is explained in further slides
- The outgoing streams also transfer some or all the equilibrated material from the Heat Exchanger module to another unit

Heat Exchanger– Outgoing streams (reaction products)

Change the local units when printing the content of this stream in its Excel worksheet

The Heat Exchanger dialog box has the following settings:

- Description: No Description
- Incoming Streams: Input 2
- Outgoing Streams:
 - Products 1: (highlighted with a red box)
 - Products 2:
- Excel Link Equation:
 - Temperature difference (C): 10
 - Temperature Change (C): [empty]
 - Enthalpy Change (J): [empty]
- Other options: Skip if No Reactants (unchecked)



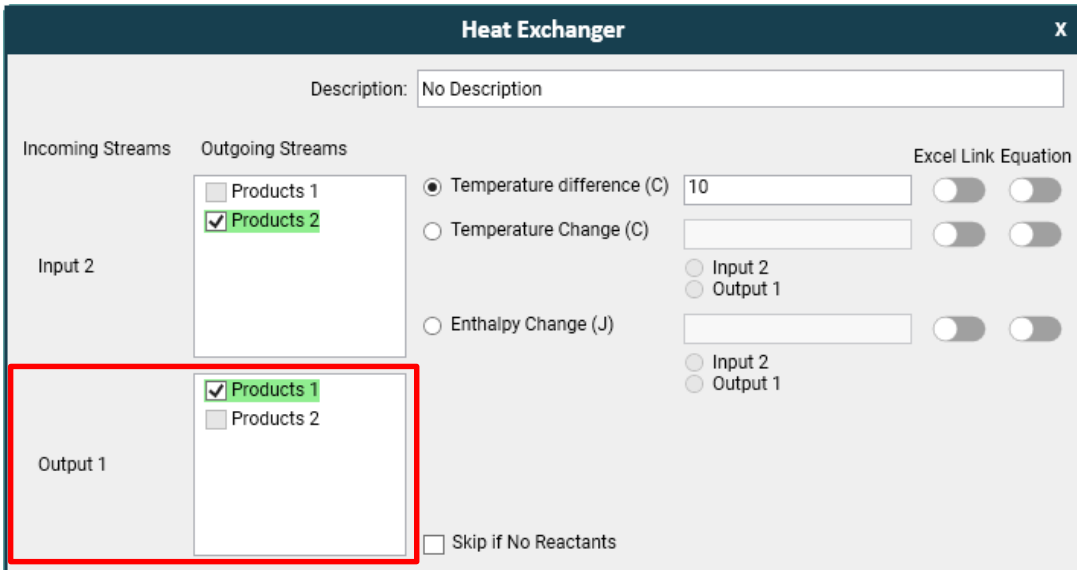
The Stream dialog box shows the following configuration:

- Description: No Description
- Name: Products 1
- Units for Printing: [Red box highlighting the button]
- Gas Phase Species:
 - 0
 - O2
 - O3
- Solution Phases:
 - BCC_A2
 - Slag-liq
 - Monoxide#1
 - Monoxide#2
 - Fe-liq
- Pure Solids:
 - Mg_solid(s)
 - Si_solid(s)
 - Ca_Solid_Alpha(s)
 - CaSi2_hR18-R3m(s)
 - Ca2Si_oP12-Pnma(s)
 - MgO_periclase(s)
 - SiO2_Quartz(l)(s)
 - SiO2_Tridymite(h)(s4)
 - SiO2_Cristobalite(h)(s6)
 - CaO_Lime(s)
- Total Selection: 0
- OK button

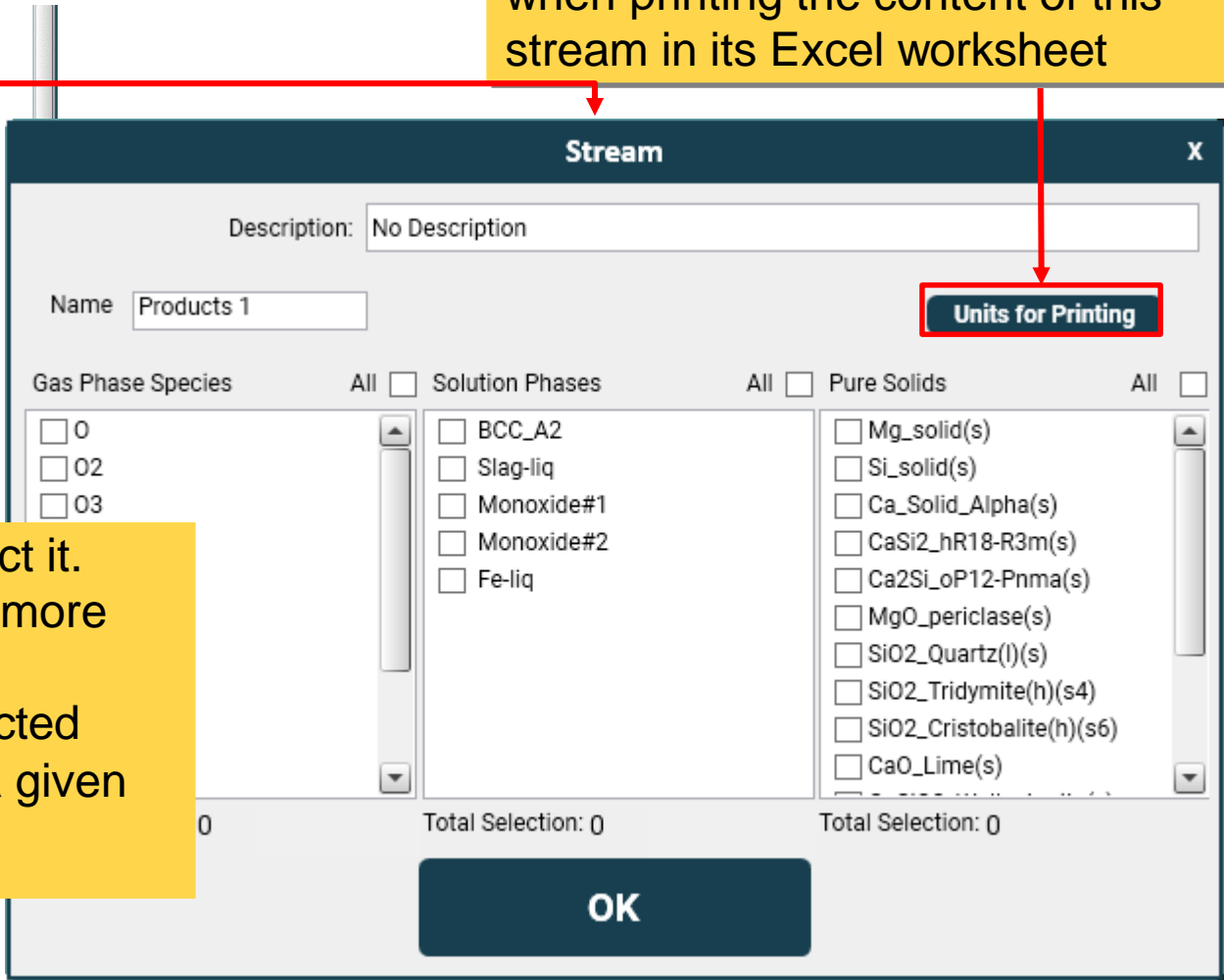
- The available phases are automatically populated from the selected database file, based on the components from its corresponding Incoming stream
- Here the phases inside the “Products 1” outgoing stream is populated based on the components from “Output 1”
- To assign Outgoing Stream to an incoming stream just click on the corresponding checkbox
- Once a outgoing stream is assigned to an incoming stream it becomes unavailable to the other stream and greyed out
- More than one outgoing stream can be assigned to incoming streams

Heat Exchanger– Outgoing streams (reaction products)

[Change the local units](#)
when printing the content of this
stream in its Excel worksheet



The Heat Exchanger dialog box shows configuration for outgoing streams. Under 'Output 1', 'Products 1' is selected with a checkbox. The 'Excel Link Equation' section has three radio buttons: 'Temperature difference (C)' (selected), 'Temperature Change (C)', and 'Enthalpy Change (J)'. The 'Temperature difference (C)' value is set to 10. There are also 'Input 2' and 'Output 1' radio buttons for each equation type.



The Stream dialog box shows configuration for 'Products 1'. It has three columns of checkboxes for species selection: 'Gas Phase Species', 'Solution Phases', and 'Pure Solids'. Each column has an 'All' checkbox. The 'Units for Printing' button is highlighted with a red box. The 'OK' button is at the bottom.

- Use the checkbox in front of the species or phase to select it. Multiple phases and species can be selected throughout more than 1 category
- ⚠ at least 1 species, solution or pure solid must be selected
- Use the 'All' checkbox to select all species or phases in a given category

Heat Exchanger– Outgoing streams (reaction products)

The image displays a software interface for a heat exchanger simulation. On the left, a control panel shows 'Incoming Streams' and 'Outgoing Streams'. The 'Outgoing Streams' section has checkboxes for 'Products 1', 'Products 2', and 'Products 3', with 'Products 1' and 'Products 3' checked. A central diagram shows a heat exchanger unit with three outgoing streams labeled 'Products 1', 'Products 2', and 'Products 3'. Two 'Stream' configuration windows are overlaid on the right. The top window is for 'Products 3' and shows 'Gas Phase Species' with checkboxes for Fe, C, C2, C3, C4, and C5, all of which are checked. The bottom window is for 'Products 1' and shows 'Gas Phase Species' with checkboxes for Fe, C, C2, C3, C4, and C5, all of which are unchecked. It also shows 'Solution Phases' with checkboxes for BCC_A2 and Fe-liq, where Fe-liq is checked. A yellow callout box with arrows pointing to the 'Fe-liq' checkbox and the 'C' checkbox in the 'Products 1' window contains the text: 'These phases cannot be selected in this stream since they are already selected in the other connected stream'.

- The outgoing streams connected to the same Incoming streams are linked: once a species, solution phase or pure solid is selected in one outgoing stream, the same species, solution phase or pure solid cannot be selected in another outgoing stream
- It is not necessary to match the entire phase selection available. However, the unselected phases will not be part of the equilibrium condition

Heat Exchanger– Outgoing streams (reaction products)

The image displays a software interface for a heat exchanger simulation. On the left, a 'Stream' dialog box shows 'Incoming Streams' and 'Outgoing Streams'. The 'Outgoing Streams' section has checkboxes for 'Products 1', 'Products 2', and 'Products 3', with 'Products 1' and 'Products 3' checked. In the center, a process flow diagram shows a heat exchanger with two outgoing streams, 'Products 3' and 'Products 1', both highlighted with red boxes. On the right, two 'Stream' dialog boxes are shown. The top one is for 'Products 3' and the bottom one is for 'Products 1'. The 'Products 3' dialog has 'Gas Phase Species' checked, with a list including Fe, C, C2, C3, C4, and C5. The 'Products 1' dialog has 'Pure Solids' checked, with a list including BCC_A2, Fe-liq, and C_Graphite(s). A yellow callout box with red arrows pointing to the 'Fe-liq' checkbox in the 'Products 1' dialog contains the text: 'These phases cannot be selected in this stream since they are already selected in the other connected stream'.

Phase Selection:

- The final Equilibrium state of the incoming stream is defined by the phases selected inside its linked outgoing streams
- The equilibrium calculation of the incoming stream will add all the phases in all the outgoing stream and incorporate them
- Here the Gas Phase and Fe-liq from “Products 1” and FCC_A1 from “Products 3” will all be added for equilibrium calculation of “Input 2”

These phases cannot be selected in this stream since they are already selected in the other connected stream

Description of the program

- Overview of the main window and commands in the Toolbar
- Step 1: Create and load a database file
- Step 2: Build the Process Flowsheet
 - Modules Panel
 - Input Stream module
 - Splitter module
 - Equilib module
 - Heat Exchanger module
 - **Using Excel Links in the modules**
 - Using Equations in the modules
 - Transferring material to the next step
 - Changing global and local units
 - Manage Splitter and Equilib Process IDs
 - Align the process modules in the flowsheet
 - Save and load an existing flowsheet
- Step 3: Check the modules – The Initializer
- Step 4: Run the process flowsheet
- Step 5: View the Results (Output Excel File)

Using Excel links – single field

- Some fields can be connected to cells in an Excel worksheet using the Excel Link option
- To activate the link for a given field, click the toggle button next to the field
- A browse window opens. Locate and select the Excel file on your computer and click Open

Local Units

Name: Input

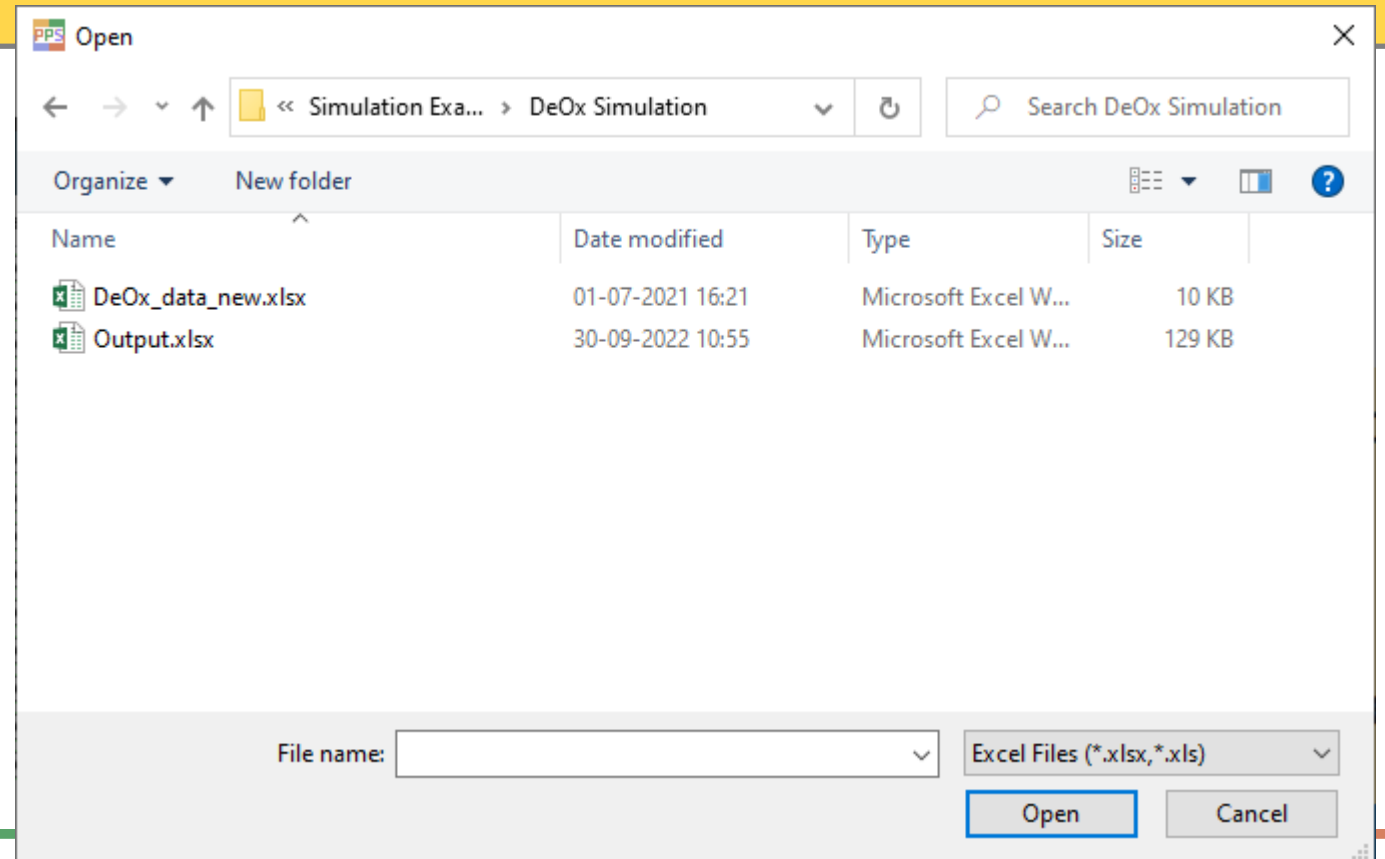
Temperature (C): 1200

Amount (kg): 20

Pressure (atm): 1

Components: ADD

Mass Percent	Species
50	CaO
30	SiO2
20	MgO



💡 Note that, in the same module, Excel links can be used for some fields, while manual entry or Equation can be used in other fields

Using Excel links – single field (continued)

Name of the current Workbook
(Excel file)

Excel Window

Workbook: D:\Projects\PyProSim\Project Plan and Presentation\LF_2023\LF_2023_ChemApp_Dofa...xlsx

Sheet: Materials

Take Value from only one cell

Initial steel		Composition (wt%)							
total amount, g	temperature (°C)	Fe	Al	C	Ca	Cr	Cu	Mn	
165000000	1600	99.7480	0.0010	0.0400	0.0000	0.0000	0.0000	0.0000	

Initial slag		Composition (wt%)						
total amount, g	temperature (°C)	Al2O3	CaO	Cr2O3	MgO	MnO	P2O5	
4950000	1600	32	51.5	0	8	0.8	0.1	
		Al2O3	CaO	Cr2O3	MgO	MnO	P2O5	
	Normalized with CaS:	31.93	51.38	0.00	7.98	0.80	0.10	

Initial inclusions		Composition (wt%)					
fraction (ppm)		Al2O3	CaO	MgO	SiO2	TiO2	MnO
1		100					

Slag formers		Composition (normalized, wt%)						
Code	Type	CaO	Al2O3	SiO2	FeO	MnO	MgO	
Lim	Lime	93.3	1	2.4	0.3	0	2.9	
None	-	NA	NA	NA	NA	NA	NA	
None	-	NA	NA	NA	NA	NA	NA	
None	-	NA	NA	NA	NA	NA	NA	
None	-	NA	NA	NA	NA	NA	NA	

OK

Navigate the worksheets in the selected Excel file, the name of the current sheet is also shown besides it

- An Excel window opens with the content of each worksheet in the selected Excel file (without formulas and formatting) in a table format
- Click in the desired cell to indicate which cell address to take the value from
- At the right-hand corner of the window, select the checkbox to indicate whether the cell address is fixed. If checked, the same cell address will be used even with multiple step simulation. If unchecked, the cell row will be incremented at each step
- **⚠ Empty cells and cells containing text instead of numbers are converted to 0**

Using Excel links – single field (continued)

Local Units Description:

Excel Link Equation

Name

Temperature (C) Check Sched

Amount (kg) Check Sched

Pressure (atm) Check Sched

Components

Mass Percent	Species
<input type="text" value="95"/>	<input type="text" value="Fe"/>
<input type="text" value="4"/>	<input type="text" value="C"/>
<input type="text" value="0.5"/>	<input type="text" value="Mn"/>
<input type="text" value="0.5"/>	<input type="text" value="Si"/>

Total%: 100

- When the value from the Excel cell is successfully read, the value is entered in the field and becomes non-editable. The toggle button is on (dark background)
- When the Excel Link is on, the value of the field will be updated with the value stored at the cell address in the Excel file every time the module is opened and at each call of that module during run
- If the cell in the Excel file contains a formula, the latter is always re-evaluated and the field is updated with the re-evaluated value
- **⚠ The program keeps the original cell address: if the user inserts or deletes columns/rows, or moves the cell in the Excel file, the program will not consider these changes. If cell address changes are made in the Excel file, the Excel link must be removed and created again**
- To remove the Excel Link, click again on the toggle button (light grey background). The field becomes editable

Using Excel links – fixed vs. variable cell address

Excel Window

Workbook: D:\Projects\PyProSim\Project Plan and Presentation\BOF 2024\Data_BOF_Simulation.xlsx

Sheet: Sheet1

Take Value from only one cell

Time (min)	O2 (kg)	CaO (kg)	Metal (A,%)	Gas (B,%)	Slag (C,%)	Scrap (kg)
1	0.57	0.25	10	50	50	2
2	0.57	0.25	10	50	50	2
3	0.57	0.25	10	50	50	2
4	0.57	0.25	10	50	50	2
5	0.57	0.25	10	50	50	2
6	0.57	0.25	10	50	50	2
7	0.57	0.25	10	50	50	2
8	0.57	0.25	10	50	50	2
9	0.57	0.25	10	50	50	2
10	0.57	0.25	30	80	80	0
11	0.57	0	30	80	80	0
12	0.57	0	30	80	80	0
13	0.57	0	30	80	80	0
14	0.57	0	30	80	80	0
15	0.57	0	30	80	80	0

Time	Temperature	Amount	Pressure
1	1300	0.25	1
2	1300	0.25	1
3	1300	0.25	1
4	1300	0.25	1
5	1300	0.25	1
6	1300	0.25	1
7	1300	0.25	1
8	1300	0.25	1
9	1300	0.25	1
10	1300	0.25	1

The value is taken from the same cell at each step

Excel Window

Workbook: D:\Projects\PyProSim\Project Plan and Presentation\BOF 2024\Data_BOF_Simulation.xlsx

Sheet: Sheet1

Take Value from only one cell

Time (min)	O2 (kg)	CaO (kg)	Metal (A,%)	Gas (B,%)	Slag (C,%)	Scrap (kg)
1	0.57	0.25	10	50	50	2
2	0.57	0.25	10	50	50	2
3	0.57	0.25	10	50	50	2
4	0.57	0.25	10	50	50	2
5	0.57	0.25	10	50	50	2
6	0.57	0.25	10	50	50	2
7	0.57	0.25	10	50	50	2
8	0.57	0.25	10	50	50	2
9	0.57	0.25	10	50	50	2
10	0.57	0.25	10	50	50	2
11	0.57	0	30	80	80	0
12	0.57	0	30	80	80	0
13	0.57	0	30	80	80	0
14	0.57	0	30	80	80	0
15	0.57	0	30	80	80	0

Time	Temperature	Amount	Pressure
1	1300	0.25	1
2	1300	0.25	1
3	1300	0.25	1
4	1300	0.25	1
5	1300	0.25	1
6	1300	0.25	1
7	1300	0.25	1
8	1300	0.25	1
9	1300	0	1
10	1300	0	1
11	1300	0	1
12	1300	0	1
13	1300	0	1
14	1300	0	1
15	1300	0	1

The cell address shifts down at each step (the column is read starting from the specified cell)

- When using multiple steps, the same cell in the Excel file can be used at each step (fixed cell address), or the cell address can be shifted at each step (variable cell address)
- ⚠ It is strongly recommended to open the schedule window after creating the Excel links to check that the values are read correctly

OK

Using Excel links – Entering components (Input Stream)

The components and their content is entered in the module, their fields cannot be edited

The components and their composition will be updated by the values from the selected cell addresses in the Excel file at each opening of the module and during run

⚠ Do not alter the cell addresses in the Excel file as the program cannot track modifications in the cell addresses in the original Excel file. If cell addresses are modified, the Excel link must be removed and created again

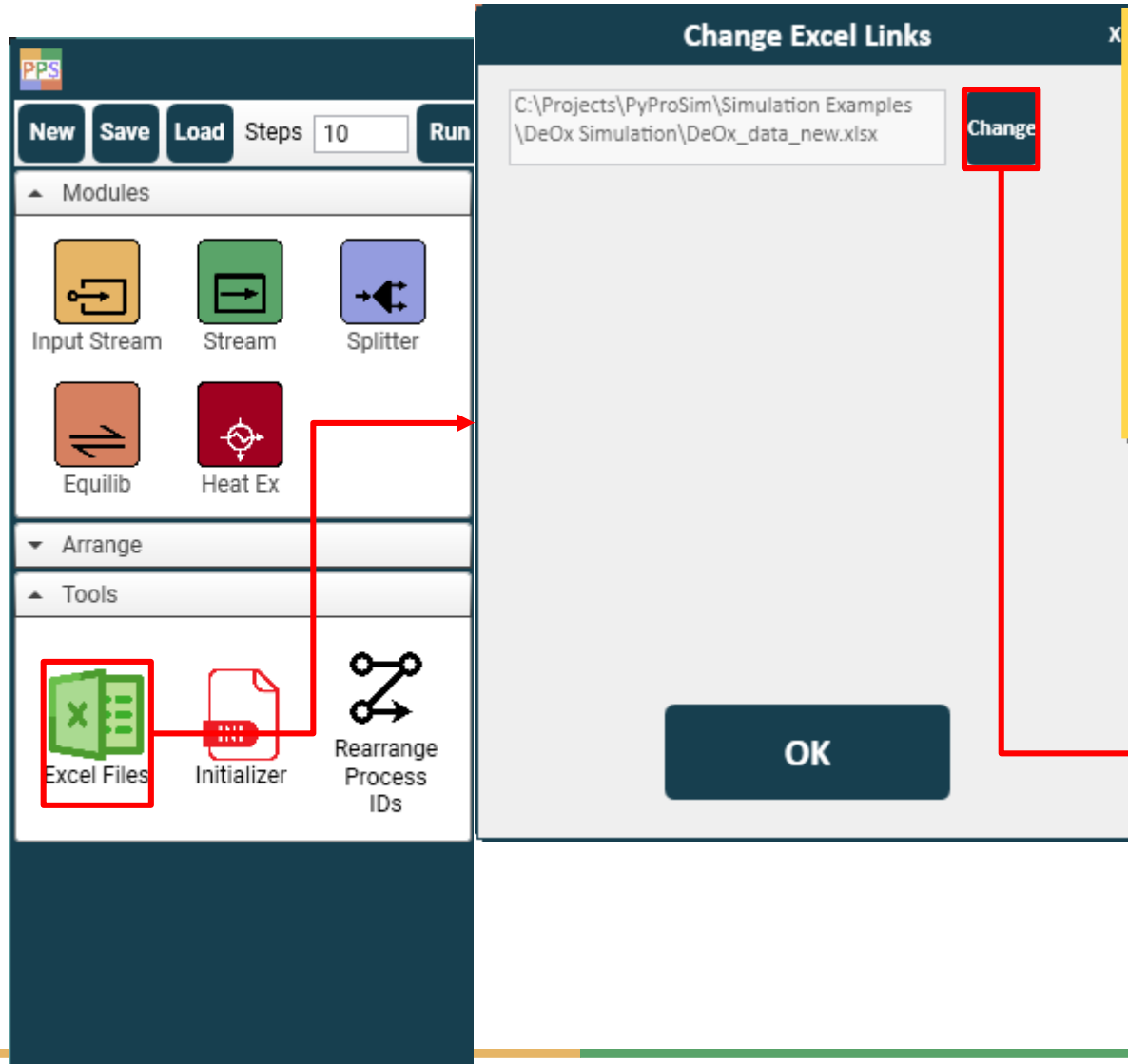
⚠ Additional components cannot be added manually

The screenshot shows the 'Local Units' configuration panel. The 'Name' field is set to 'Input'. There are three 'Check Sched' options for Temperature (C), Amount (kg), and Pressure (atm), each with a toggle switch. The 'Components' section is highlighted with a red box and contains an 'ADD' button and a toggle switch. Below this is a table with two columns: 'Mass Percent' and 'Species'. The table contains four rows of data: Fe (95%), C (4%), Mn (0.5%), and Si (0.5%). The total mass percent is 100%.

Mass Percent	Species
95	Fe
4	C
0.5	Mn
0.5	Si

Total%: 100

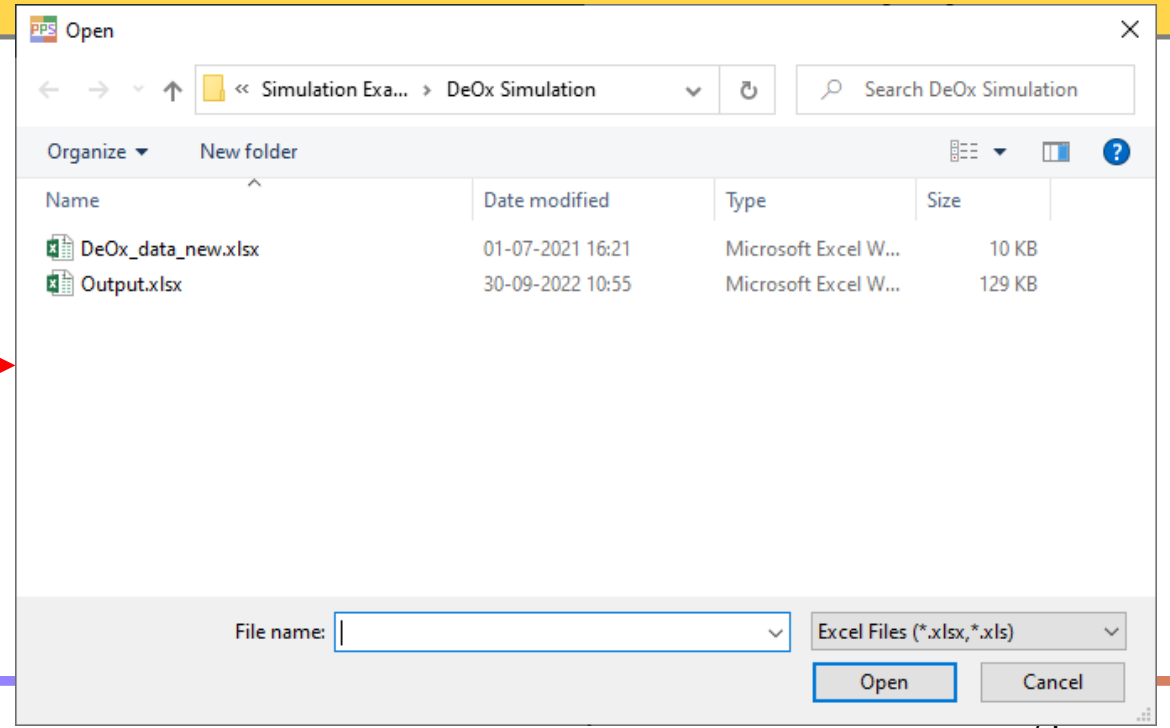
Using Excel links – Changing the Excel file(s)



When using Excel links in modules, the name and location of the Excel source files is stored with the flowsheet. It can be viewed and changed using the Excel Files button in the Tools Panel

Press the Change button next to the Excel file path to open a browse window and select a different Excel file

⚠ Cell addresses provided in the modules are unchanged



Using Excel links – Reviewing the selection

Local Units Description:

Excel Link Equation

Name

Temperature (C) Check Sched

Amount (kg) Check Sched

Pressure (atm) Check Sched

Components **ADD**

Mass Percent Species

<input type="text" value="95"/>	<input type="text" value="Fe"/>
<input type="text" value="4"/>	<input type="text" value="C"/>
<input type="text" value="0.5"/>	<input type="text" value="Mn"/>
<input type="text" value="0.5"/>	<input type="text" value="Si"/>

Total%: 100

Excel Window

Workbook: D:\Projects\PyProSim\Project Plan and Presentation\BOF 2024\Data_BOF_Simulation.xlsx

Sheet: Sheet1 Take Value from only one cell

Scrap	100					25					
Time (min)	O2 (kg)	CaO (kg)	Metal (A,%)	Gas (B,%)	Slag (C,%)	Scrap (kg)	dH (kJ)	0			
1	0.57	0.25	10	50	50	2					
2	0.57	0.25	10	50	50	2					
3	0.57	0.25	10	50	50	2					
4	0.57	0.25	10	50	50	2					
5	0.57	0.25	10	50	50	2					
6	0.57	0.25	30	80	80	2					
7	0.57	0.25	30	80	80	2					
8	0.57	0.25	30	80	80	2					
9	0.57	0.25	30	80	80	2					
10	0.57	0.25	30	80	80	0					
11	0.57	0	30	80	80	0					
12	0.57	0	30	80	80	0					
13	0.57	0	30	80	80	0					
14	0.57	0	30	80	80	0					
15	0.57	0	30	80	80	0					

- After connecting to Excel, the “i” option will become active
- This option will show the selection made during connection and further modification can be made if necessary
- ⚠ The program keeps the original cell address: if the user inserts or deletes columns/rows, or moves the cell in the Excel file, the program will not consider these changes. If cell address changes are made in the Excel file, the Excel link must be removed and created again

Description of the program

- Overview of the main window and commands in the Toolbar
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- Step 5: View the Results (Output Excel File)

Using Equation

Local Units

Description: No Description

Excel Link

Equation

Gas Phase Species

- Si
- Si2
- Si3
- C
- C2
- C3
- C4
- C5
- SiC
- SiC2
- Si2C
- Mn
- Fe

Components

ADD

Mass Percent

Mass Percent	Species
95	Fe
4	C
0.5	Mn
0.5	Si

Total%: 100

- Some fields can be connected to an Equation using the Equation option
- To activate the link for a given field, click the toggle button next to the field
- An Equation Builder window will open, where you can define your Equation

💡 Note that, in the same module, Equations can be used for some fields, while manual entry or Excel link can be used in other fields

Equation Builder

Sample function (Fn) = $3*2 + 5*[var1] - ([var2] + 7*[var3])$

Fn = 3*2

+ VAR - VAR AUTO Help

Name Excel Stream

OK

Using Equation

Equation Area: Write your equation here

Equation Builder

Sample function (Fn) = $3*2 + 5*[var1] - ([var2] + 7*[var3])$

Fn =

Name	Excel	Stream
<input type="text" value="a"/>	<input type="checkbox"/>	<input type="text"/>
<input type="text" value="var2"/>	<input type="checkbox"/>	<input type="text"/>
<input type="text" value="metal"/>	<input type="checkbox"/>	<input type="text"/>

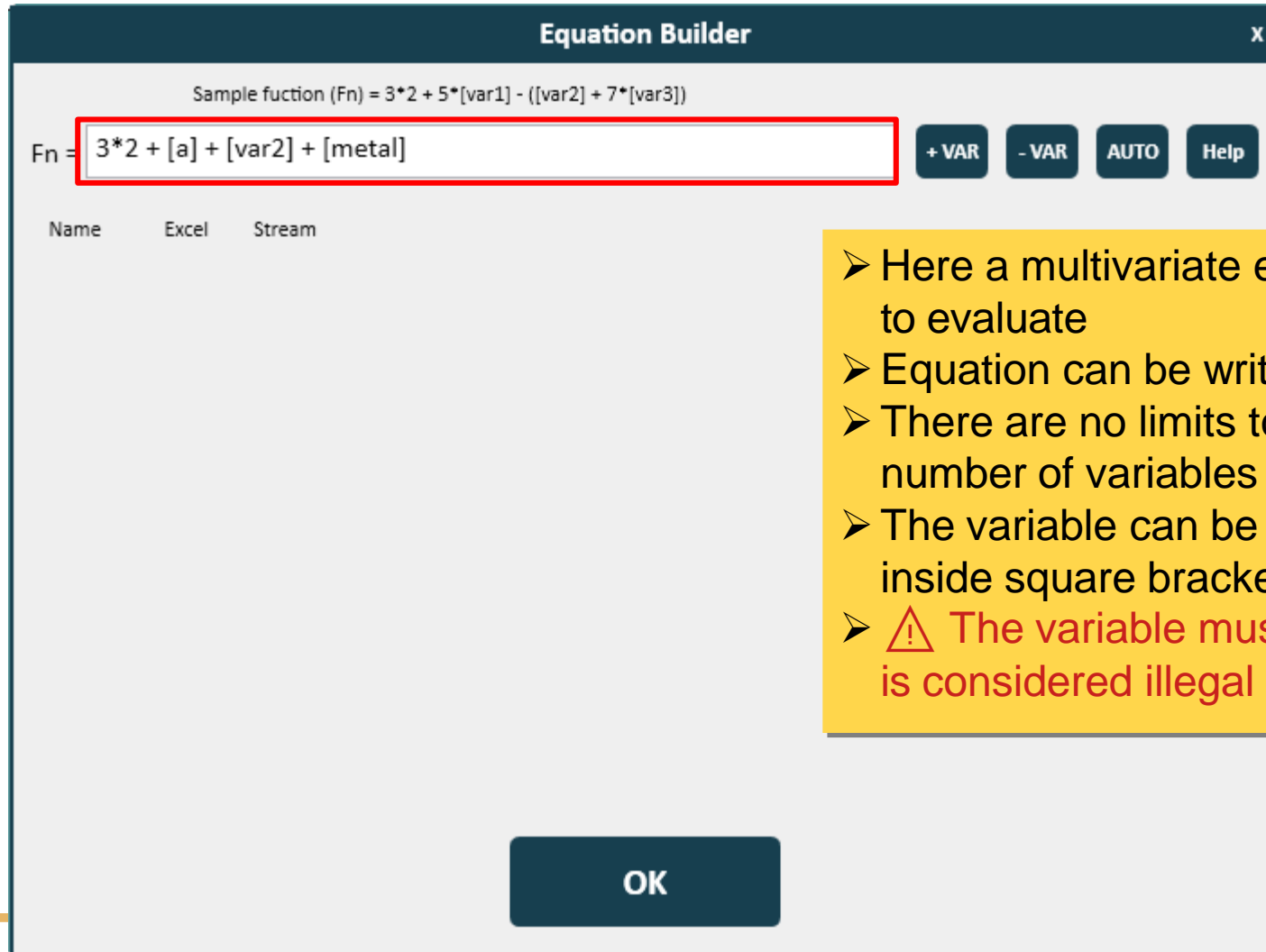
Variable Area: All the variables will be shown here, which then can be defined

- **+VAR** will add a single variable to the Variable Area
- **-VAR** will remove the selected variable from the Variable Area

💡 These two options will only generate variables with generic name, user need to rewrite the name according to equation variables

- **AUTO** will read the equation in the *Equation Area*, identifies the written variables in the equation and then populate the *Variable Area* with corresponding variables
- **Help** will open this user manual

Using Equation: Equation Text



- Here a multivariate equation can be written for the FactProSim to evaluate
- Equation can be written in the form similar to Excel
- There are no limits to the length of the equation and the number of variables used
- The variable can be named anything as long as they are written inside square brackets [..]
- ⚠ The variable must be written inside [..], anything outside is considered illegal and a warning will be generated

Using Equation: Variable declarations

The screenshot shows the 'Equation Builder' window with the following components:

- Equation: $F_n = 3 \cdot 2 + [a] + [var2] + [metal]$
- Buttons: + VAR, - VAR, AUTO, Help
- Variable Declaration Table:

Name	Excel	Stream
a	<input checked="" type="checkbox"/>	<input type="text"/>
var2	<input type="checkbox"/>	<input type="text"/>
metal	<input type="checkbox"/>	<input type="text"/>

The 'Excel' column for 'a' is highlighted with a red box, and a red arrow points from this box to a callout box below. The 'Stream' column for 'a' is also highlighted with a red box.

➤ The variables will be shown in the Variable area where they will be defined

➤ The value of the variable can be linked to Excel, ([as shown here](#))

- FactProSim evaluates the variable value at each time step
- The variable value can be defined in two ways:
 - Using Excel
 - Manually connecting the value to an existing Input Stream or Stream
- When the value from the Excel is linked, all the other field on the row will be greyed out and become inactive

Using Equation: Variable declarations

Equation Builder

Sample fuction (Fn) = $3*2 + 5*[var1] - ([var2] + 7*[var3])$

Fn =

+ VAR - VAR AUTO Help

Name	Excel	Stream
<input type="text" value="a"/>	<input type="checkbox"/>	<input type="text" value="Stream: Gas out"/>
<input type="text" value="var2"/>	<input type="checkbox"/>	<input type="text" value="Input Stream: Gas in"/>
<input type="text" value="metal"/>	<input type="checkbox"/>	<input type="text" value="Input Stream: Metal Fuel in"/>

OK

➤ A list of all the Input Streams and Streams currently part of the process model will pop out after clicking on the drop down menu

💡 Note that, it shows all streams, regardless of its connection to current module

➤ Select the desired stream from the list

Using Equation: Variable declarations

Sample function (Fn) = $3*2 + 5*[var1] - ([var2] + 7*[var3])$

Fn = $3*2 + [a] + [var2] + [metal]$

Note that, Amount, Temperature and Pressure will be evaluated directly; whereas Gas Phase, Solution Phase or Solid Phase will add more options

After selecting the desired stream another drop down menu appears

Select the field whose value you want to add to the variable

OK

OK

Using Equation: Variable declarations

Equation Builder

Sample function (Fn) = $3*2 + 5*[var1] - ([var2] + 7*[var3])$

Fn =

+ VAR - VAR AUTO Help

Name	Excel	Stream
<input type="text" value="a"/>	<input type="checkbox"/>	Input Stream: <input type="text" value="c"/>
<input type="text" value="var2"/>	<input type="checkbox"/>	<input type="text" value=""/>
<input type="text" value="metal"/>	<input type="checkbox"/>	<input type="text" value=""/>

Gas Phase

- Amount (g)
- Phase Component
- System Component

OK

- If Gas Phase is selected, it will add extra option where you can select either Amount or one of the Component
- If you select either Phase Component or System Component, they will give extra option

Using Equation: Variable declarations

The screenshot shows the 'Equation Builder' window with the equation $F_n = 3*2 + [a] + [var2] + [metal]$. Below the equation, there are three variable declarations: 'a', 'var2', and 'metal'. Each has a name field, an 'Excel' checkbox, and a 'Stream' dropdown menu. The 'Stream' menu for 'a' is open, showing 'Gas Phase' and 'Phase Compon' options. The 'Phase Compon' dropdown is also open, showing a list of options: 'O (g/g)', 'O2 (g/g)', and 'O3 (g/g)'. Buttons for '+ VAR', '- VAR', 'AUTO', and 'Help' are visible.

The screenshot shows the 'Equation Builder' window with the same equation $F_n = 3*2 + [a] + [var2] + [metal]$. The 'Stream' dropdown menu for 'a' is open, showing 'Gas Phase' and 'System Compo' options. The 'System Compo' dropdown is also open, showing a list of options: 'Fe (g/g)', 'Al (g/g)', 'O (g/g)', 'N (g/g)', 'e(Spinel#1) (g/g)', and 'e(Spinel#2) (g/g)'. Buttons for '+ VAR', '- VAR', 'AUTO', and 'Help' are visible.

- Phase Component will give the option to select End members of the phase defined in the database (.cst file)
- System Component will give the option to select Elements (Chemical Species) defined in the database (.cst) file

Using Equation: Variable declarations

Equation Builder

Sample fuction (Fn) = $3 \cdot 2 + 5 \cdot [\text{var1}] - ([\text{var2}] + 7 \cdot [\text{var3}])$

Fn = $3 \cdot 2 + [\text{a}] + [\text{var2}] + [\text{metal}]$ + VAR - VAR AUTO Help

Name	Excel	Stream
a	<input type="checkbox"/>	Input Stream: (Gas Phase Phase Compon O2 (mol/mol)
var2	<input type="checkbox"/>	Input Stream: I Solution Phase
metal	<input type="checkbox"/>	Stream: Oxidis

LIQUID#1
LIQUID#2
FCC_A1#1
FCC_A1#2
FCC_A1#3
BCC_A2#1
BCC_A2#2
HCP_A3#1
HCP_A3#2
Me4N#1
Me4N#2
BCC_B2#1
BCC_B2#2
Al13Fe4
Al8Fe5#1
Al8Fe5#2
Slag-liq#1
Slag-liq#2

➤ If Solution Phase is selected it will add extra option, where you can select any solution phase **except** Gas Phase

Using Equation: Variable declarations

Equation Builder

Sample fuction (Fn) = $3*2 + 5*[var1] - ([var2] + 7*[var3])$

Fn = + VAR - VAR AUTO Help

Name	Excel	Stream	Phase	Component	Unit
a	<input type="checkbox"/>	Input Stream: t	Gas Phase	Phase Compon	O2 (mol/mol)
var2	<input type="checkbox"/>	Input Stream: l	Solution Phase	LIQUID#2	
metal	<input type="checkbox"/>	Stream: Oxidisi			

Amount (g)
Phase Component
System Component

OK

- After phase selection it will add extra option, where you can select either Amount or one of the Component
- If you select either Phase Component or System Component, they will give extra option

Using Equation: Variable declarations

The screenshot shows the 'Equation Builder' window with the equation $F_n = 3 \cdot 2 + [a] + [\text{var2}] + [\text{metal}]$. Below the equation, there are three variable declarations:

Name	Excel	Stream
a	<input type="checkbox"/>	Input Stream: <input type="text"/> Gas Phase Phase Compon O2 (mol/mol)
var2	<input type="checkbox"/>	Input Stream: <input type="text"/> Solution Phase LIQUID#2 Phase Compon <input type="text"/>
metal	<input type="checkbox"/>	Stream: Oxidis <input type="text"/>

A dropdown menu is open for the 'Phase Compon' field of 'var2', showing options: Al (g/g), Fe (g/g), N (g/g), and O (g/g). An 'OK' button is visible at the bottom.

The screenshot shows the 'Equation Builder' window with the same equation $F_n = 3 \cdot 2 + [a] + [\text{var2}] + [\text{metal}]$. Below the equation, there are three variable declarations:

Name	Excel	Stream
a	<input type="checkbox"/>	Input Stream: <input type="text"/> Gas Phase Phase Compon O2 (mol/mol)
var2	<input type="checkbox"/>	Input Stream: <input type="text"/> Solution Phase LIQUID#2 System Compo <input type="text"/>
metal	<input type="checkbox"/>	Stream: Oxidis <input type="text"/>

A dropdown menu is open for the 'System Compo' field of 'var2', showing options: Fe (g/g), Al (g/g), O (g/g), N (g/g), e(Spinel#1) (g/g), and e(Spinel#2) (g/g). An 'OK' button is visible at the bottom.

- Phase Component will give the option to select End members of the phase defined in the database (.cst file)
- System Component will give the option to select Elements (Chemical Species) defined in the database (.cst) file

Using Equation: Variable declarations

Equation Builder

Sample fuction (Fn) = $3*2 + 5*[var1] - ([var2] + 7*[var3])$

Fn = $3*2 + [a] + [var2] + [metal]$ + VAR - VAR AUTO Help

Name	Excel	Stream	Phase	Compon
a	<input type="checkbox"/>	Input Stream: (Gas Phase	O2 (mol/mol)
var2	<input type="checkbox"/>	Input Stream: I	Solution Phase	LIQUID#2
metal	<input type="checkbox"/>	Stream: Oxidisi	Solid Phase	

- Al_fcc_A1(s) (g)
- Al_hcp_A3(s2) (g)
- Al_hcp_Zn(s3) (g)
- Al_cbcc_A12(s4) (g)
- Al_bcc_A2(s5) (g)
- Al_cub_A13(s6) (g)
- Al_bct_A5(s7) (g)
- Al_diamond_A4(s8) (g)
- Al_DHCP(s9) (g)
- Fe_BCC_A2(s) (g)
- Fe_FCC_A1(s2) (g)
- FeAl2_S1(s) (g)
- Fe2Al5_S1(s) (g)
- Al2O3_gamma(s) (g)
- Al2O3_delta(s2) (g)
- Al2O3_kappa(s3) (g)

- If Solid Phase is selected it will add extra option, where you can select any solid phase
- There is no other extra option in solid phase

Using Equation: Variable Unit

The screenshot displays the FactProSim software interface. The main window is the 'Equation Builder', which shows a sample function $F_n = 3 \cdot 2 + [a] + [var2] + [metal]$. Below the equation, there are three variables: 'a', 'var2', and 'metal'. Each variable has a dropdown menu for 'Stream' and 'Phase'. The 'a' variable is set to 'Input Stream: I' and 'Gas Phase'. The 'var2' variable is set to 'Input Stream: I' and 'Solution Phase'. The 'metal' variable is set to 'Stream: Oxidis' and 'Solid Phase'. A dropdown menu for 'Solid Phase' is open, showing a list of options including 'Al_fcc_A1(s) (g)', 'Al_hcp_A3(s2) (g)', 'Al_hcp_Zn(s3) (g)', 'Al_cbcc_A12(s4) (g)', 'Al_bcc_A2(s5) (g)', 'Al_cub_A13(s6) (g)', 'Al_bct_A5(s7) (g)', 'Al_diamond_A4(s8) (g)', 'Al_DHCP(s9) (g)', 'Fe_BCC_A2(s) (g)', 'Fe_FCC_A1(s2) (g)', 'FeAl2_S1(s) (g)', 'Fe2Al5_S1(s) (g)', 'Al2O3_gamma(s) (g)', 'Al2O3_delta(s2) (g)', and 'Al2O3_kappa(s3) (g)'. The 'Al_fcc_A1(s) (g)' option is selected. A 'Change Units' dialog box is open, showing options for 'Global' and 'Local' units for Temperature, Amount, Pressure, Energy, and Volume. The 'Local' units are selected for all categories. The 'Units for Printing' dialog box is also open, showing options for 'Units for Printing'.

Each evaluable option (i.e. the option which does not generate more option when selected), will have its unit written beside it

The unit depends on the unit of the module it is derived from, (the stream selected under Stream option)

⚠ If any changes to the unit is made after the variable initialization, then the selection in the equation builder becomes invalid and needs to be revisited

Using Equation: IFELSE condition

Equation Builder X

Sample fuction (Fn) = $3*2 + 5*[var1] - ([var2] + 7*[var3])$

Fn = + VAR - VAR AUTO Help

Na Format: IFELSE (V1 IF(COND), V2)

A **COND**: this is some condition which gives either true or false, for e.g. (A > 2)

B **V1**: this is the value taken if the COND is *true*

V2: this is the value taken if the COND is *false*

The statement can be nested (not recommended)
IFELSE(V1 IF(IFELSE(V3 IF(COND1), V4) > V5), V2)

In this example:
COND: [A] < [B]
V1: [A]
V2: [B]

OK

Using Equation: Supported Functions

- List of function supported:
 - All basic operation (+, -, /, *)
 - abs(number): absolute value of number
 - arccos(number): inverse of cos
 - arccosec(number): inverse of cosec
 - arccotan(number): inverse of cotan
 - arcsec(number): inverse of sec
 - arcsin(number): inverse of sin
 - arctan(number): inverse of tan
 - cbrt(number): cube root of the number
 - sqrt(number): square root of the number
 - tan(number)
 - sin(number)
 - cos(number)
 - cosec(number)
 - cotan(number)
 - arccosec(number)
 - arccotan(number)
 - ln(number): natural log of the number
 - log(x): base 10 log of x
 - log(y, x): log of x with base y
 - x^y : x raised to the power y
 - sec(number)
 - signum(number)
 - sqr(number): square of the number

Using Equation: Reviewing the selection

Local Units Description:

Excel Link Equation

Temperature (C) Check Schedu

Enthalpy (J) Check Schedu

Pressure (atm) Check Schedu

Process ID

Incoming Streams

FeTi
undisolv FeTi

Outgoing Streams

FeTi comb

Skip if No Reactants

Equation Builder X

Sample function (Fn) = $3*2 + 5*[var1] - ([var2] + 7*[var3])$

Fn = + VAR - VAR AUTO Help

Name	Excel	Stream
G	<input type="checkbox"/>	Stream: steel Amount (g)
A1	<input checked="" type="checkbox"/>	
A2	<input checked="" type="checkbox"/>	
B	<input type="checkbox"/>	Stream: Steel Temperature
C	<input checked="" type="checkbox"/>	
D	<input type="checkbox"/>	Stream: Steel Amount (g)
E	<input checked="" type="checkbox"/>	

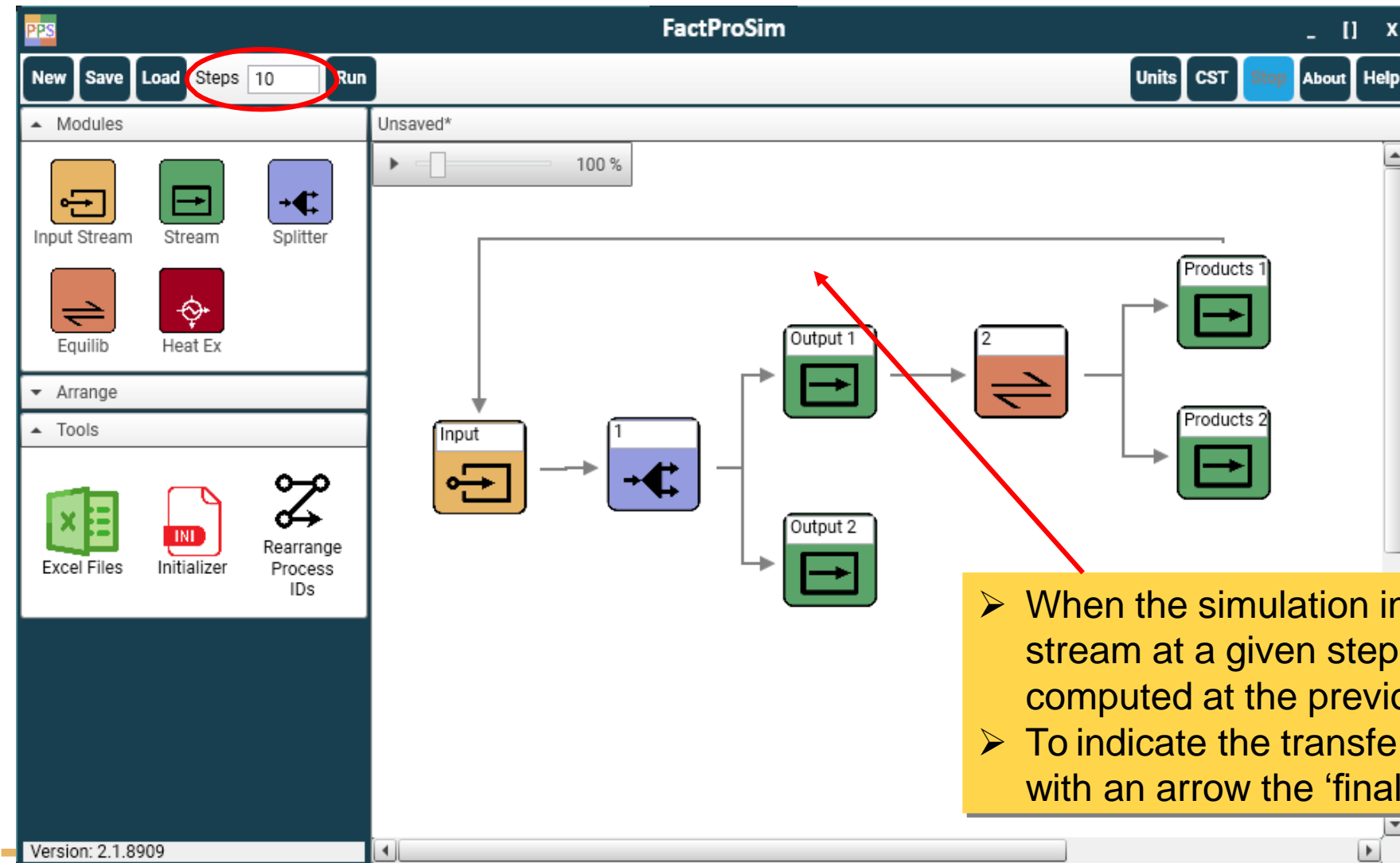
OK

- After connecting to Equation, the “i” option will become active
- This option will show the selection made during connection and further modification can be made if necessary

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 - Using Equations in the modules
 - **Transferring material to the next step**
 - Changing global and local units
 - Manage Splitter and Equilib Process IDs
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Transferring material to the next step



- When the simulation involves multiple time steps, an input stream at a given step might be associated to a stream computed at the previous step
- To indicate the transfer of stream to the next step, connect with an arrow the 'final' Stream to the Input Stream

Transferring material to the next step

Input Stream [x]

Local Units Description: No Description

Excel Link Equation Gas Phase Species All Solution Phases All Pu

Name: Input

Temperature (C): 1300

Amount (kg): 0.25

Pressure (atm): 1

Components: **ADD**

Mass Percent	Species
95	Fe
4	C
0.5	
0.5	

Total%: 100

Total Selection: 3

Total Selection: 0

OK **Schedule**

- When a connection (transfer) is made between a Stream and an Input Stream, the Input stream needs to be defined only for the 1st step (the schedule becomes unavailable)
- From the 2nd step, the Input Stream will be replaced by the connected Stream computed at the previous step. All information in the Stream is copied to the Input Stream: amount, temperature, composition and phase selection

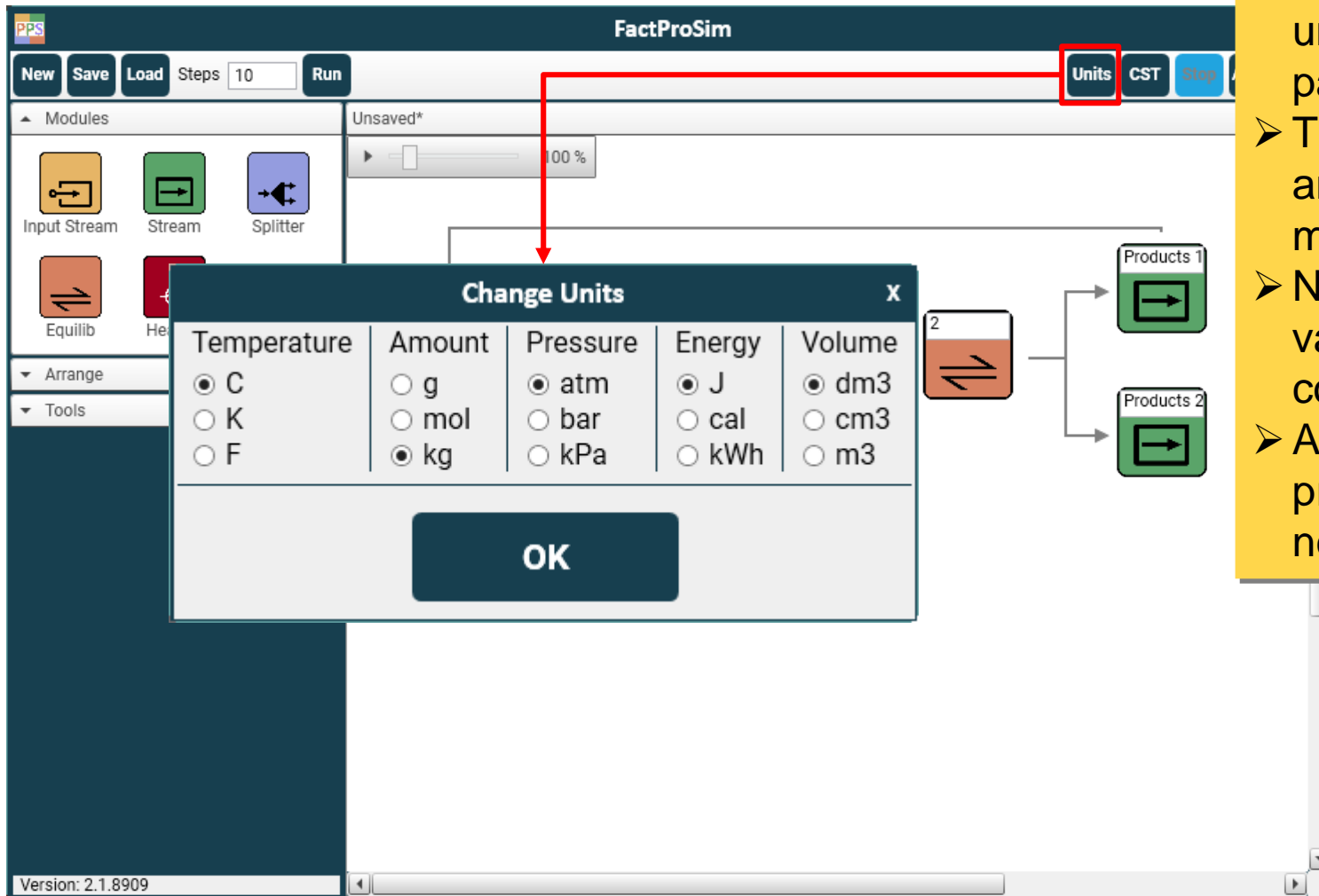
T, mass, P, composition and phase selection only applies for the 1st step

Schedule becomes unavailable

Description of the program

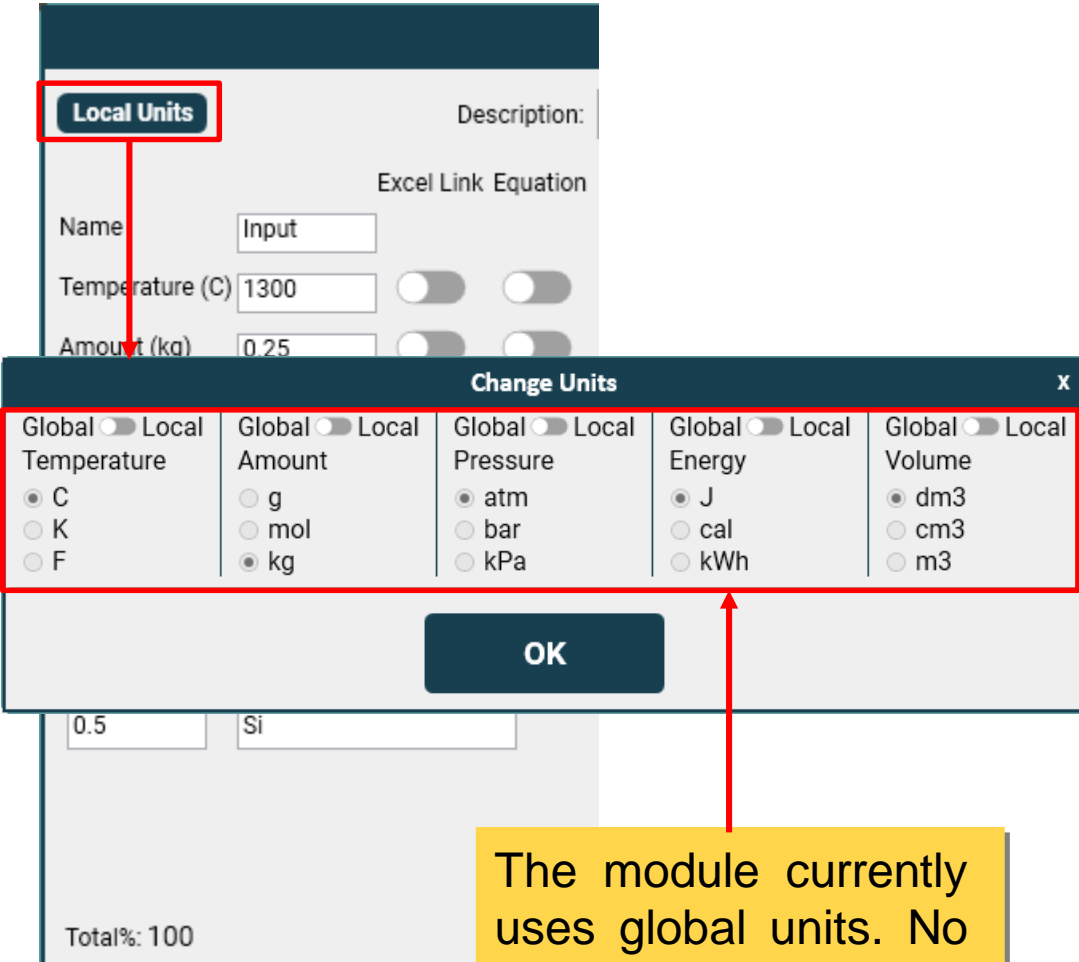
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Global Units



- The main units for the simulations, the global units, can be changed via the Global Units panel in the main window
- The change of units is applied to all modules and all printed values (except in specific modules where local units are activated)
- Note that, when changing the units, the values already entered in the modules are not converted
- Additional units for temperature, amount, pressure and enthalpy will be available in the next program version

Global and Local Units

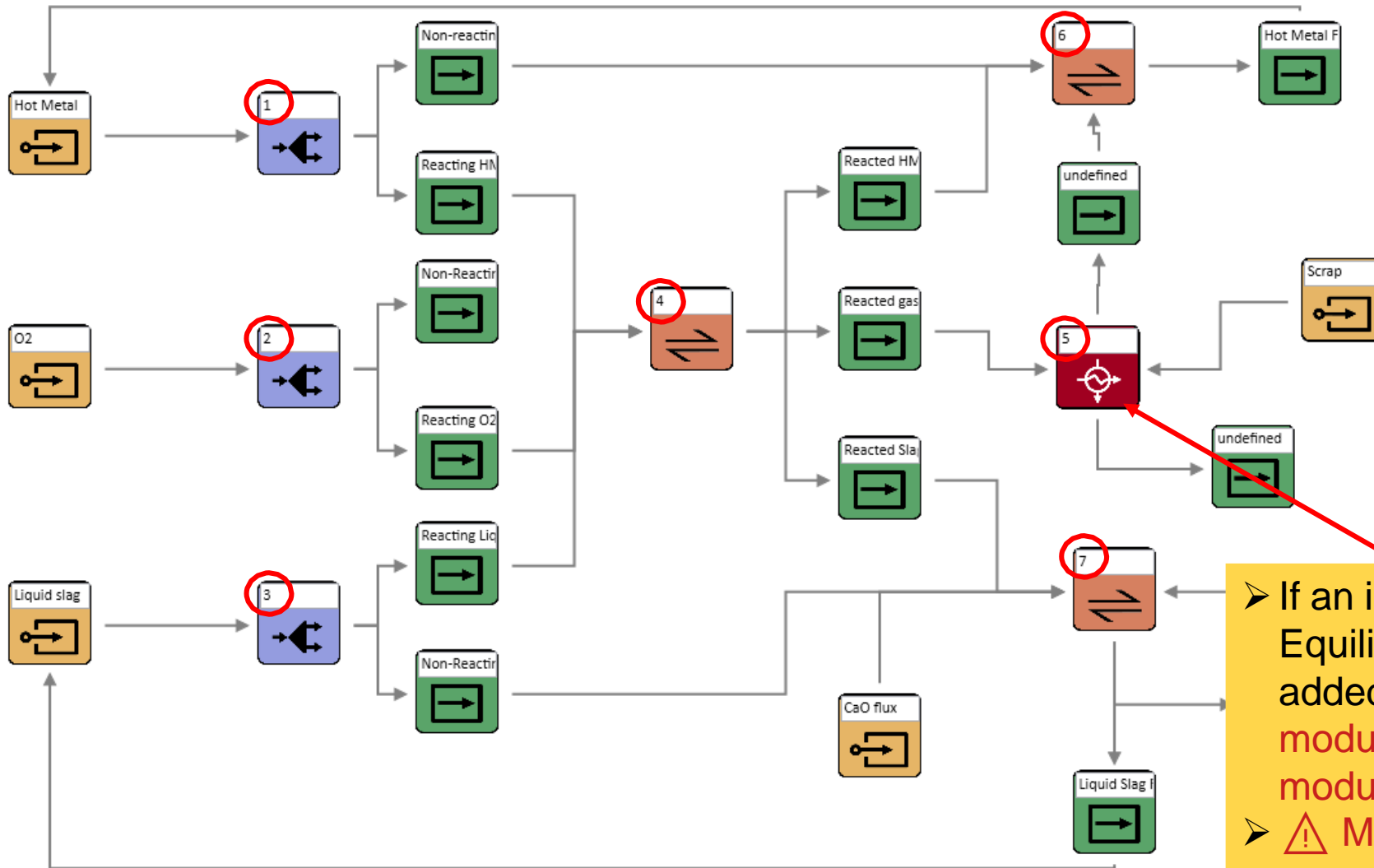


- It might be more practical to use other units than the global units in specific modules in the diagram. Therefore, Local Units can be defined in each Input Stream and Equilib module
- In the module, click the Local Units button. By default, the Units are set to Global. Use the toggle button to switch the temperature and/or the amount to Local Units. The Units selection becomes editable
- ⚠ Once Local Units are active, the local unit will remain fixed even though the Global Units are modified
- Switch back the toggle button to return to Global units

Description of the program

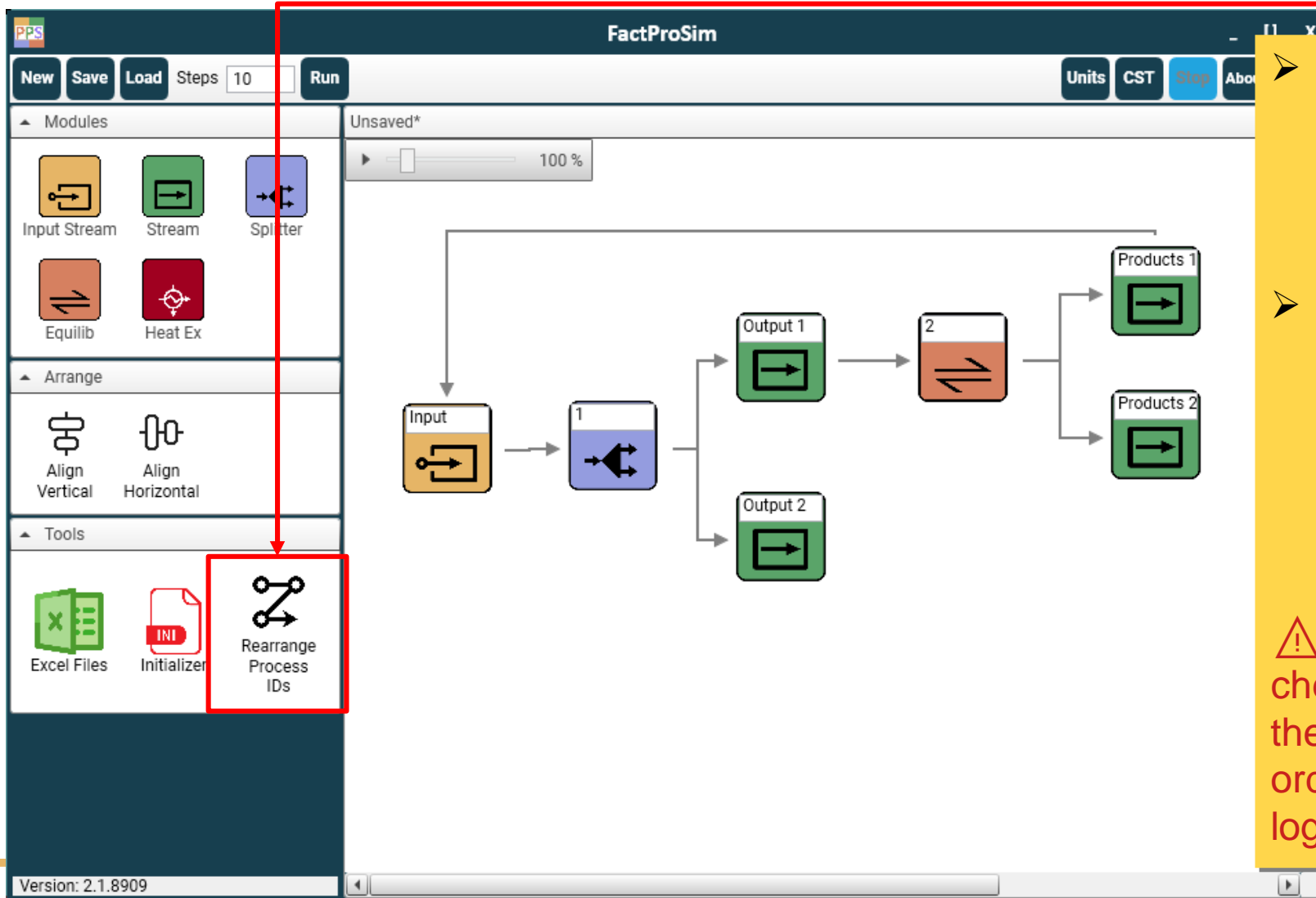
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Managing process IDs



- If an intermediate operation (splitter, Equilib or Heat Exchanger) must be added, the process ID number of the new module and those following the new module must be manually updated
- ⚠ Modules cannot have the same process IDs!

Auto arrange process IDs



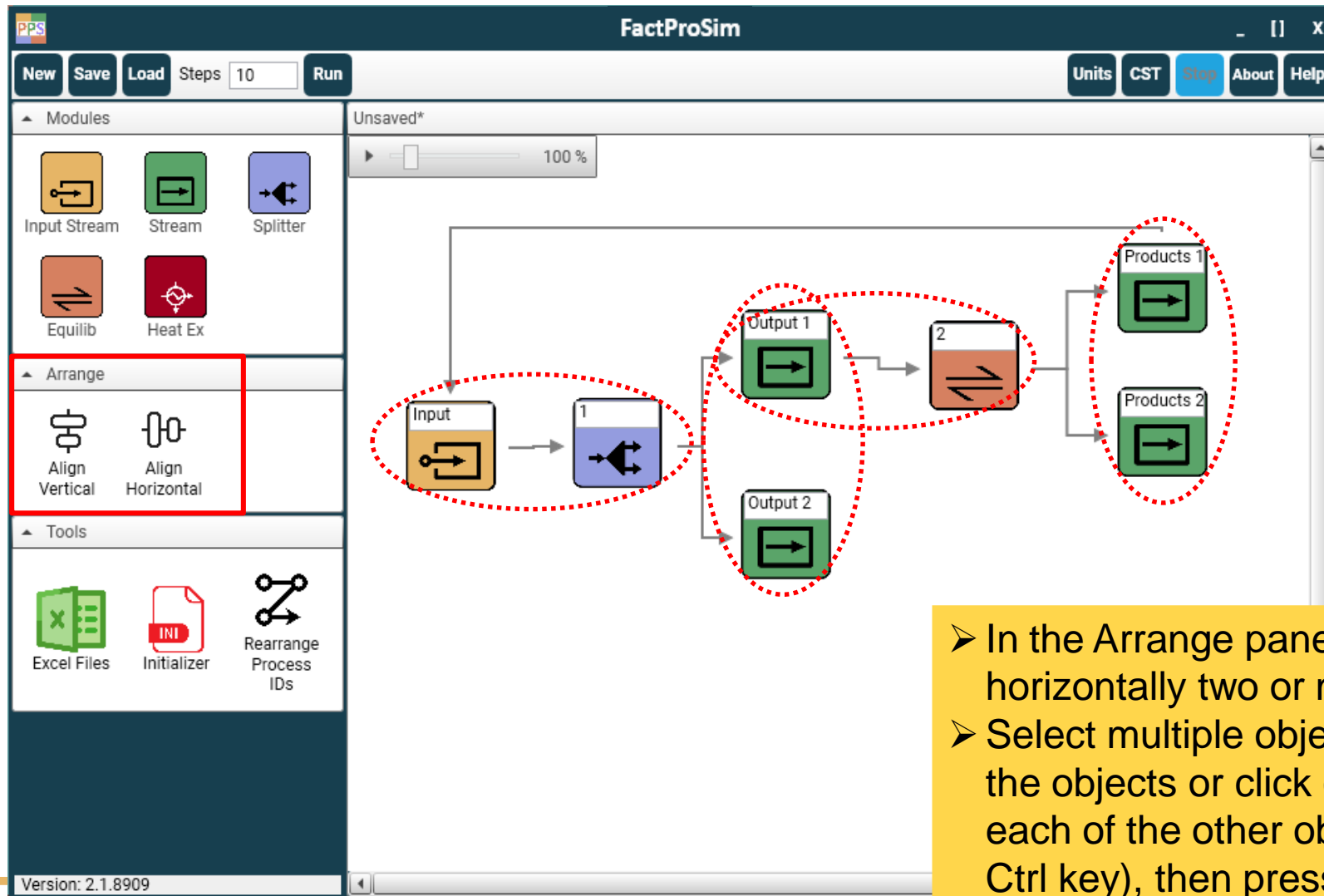
- The Rearrange Process IDs function in the Local controls panel allows to renumber process IDs to have a continuous numbering in the flowsheet
- When 2 modules have identical process ID, the module that was inserted first in the diagram will keep its process ID while the other module will be assigned the next process ID. The process IDs of all the following modules will be updated

⚠ The Rearrange Process IDs does not check if the Process ID order is logical. It is the user's responsibility to check that the order of the operations in the flowsheet is logical

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Align the modules in the diagram

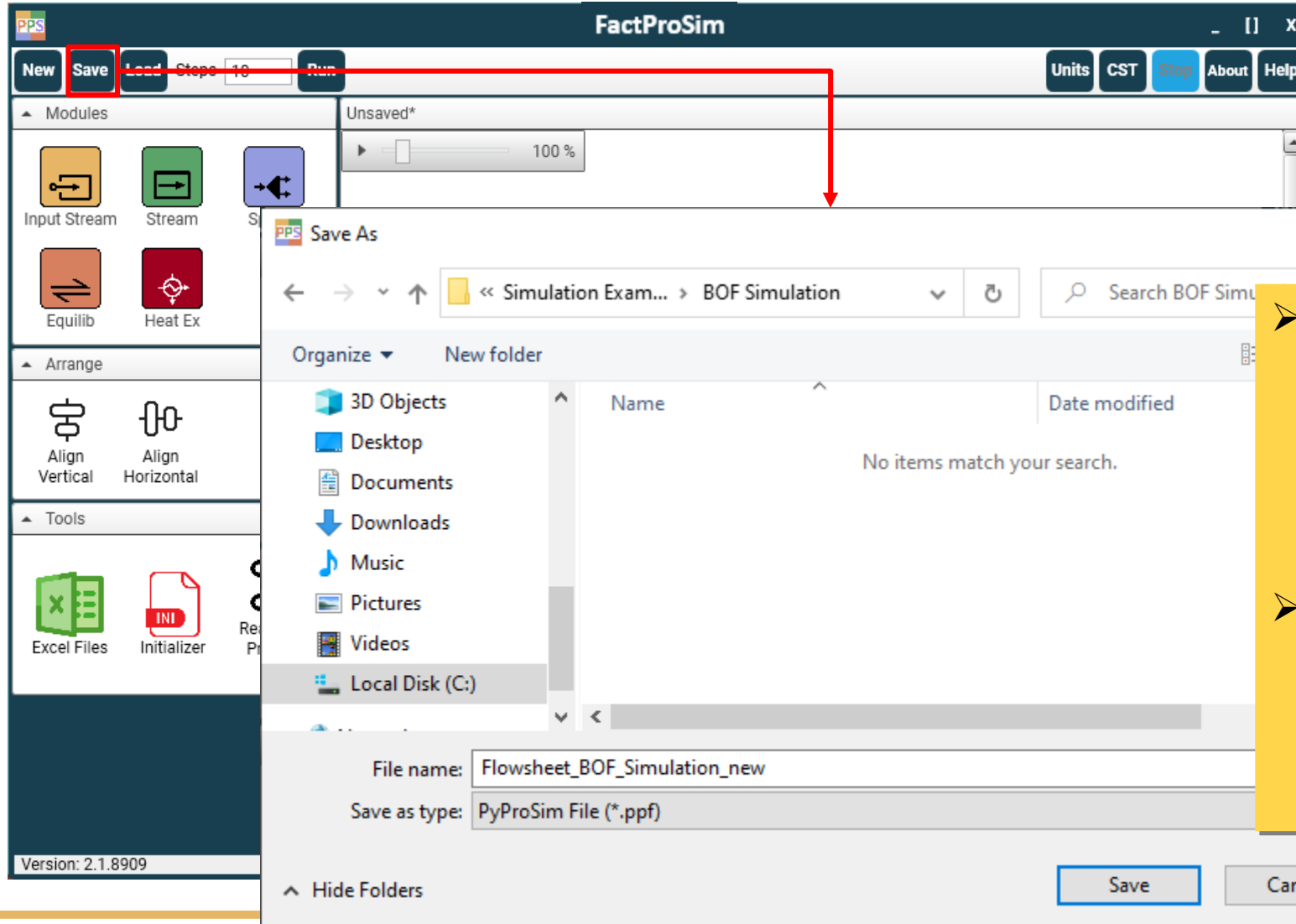


- In the Arrange panel, two buttons allow to align vertically or horizontally two or more selected objects
- Select multiple objects (either click and drag a box around the objects or click one object, press the Ctrl key and select each of the other object you want while holding down the Ctrl key), then press the button align vertical or horizontal

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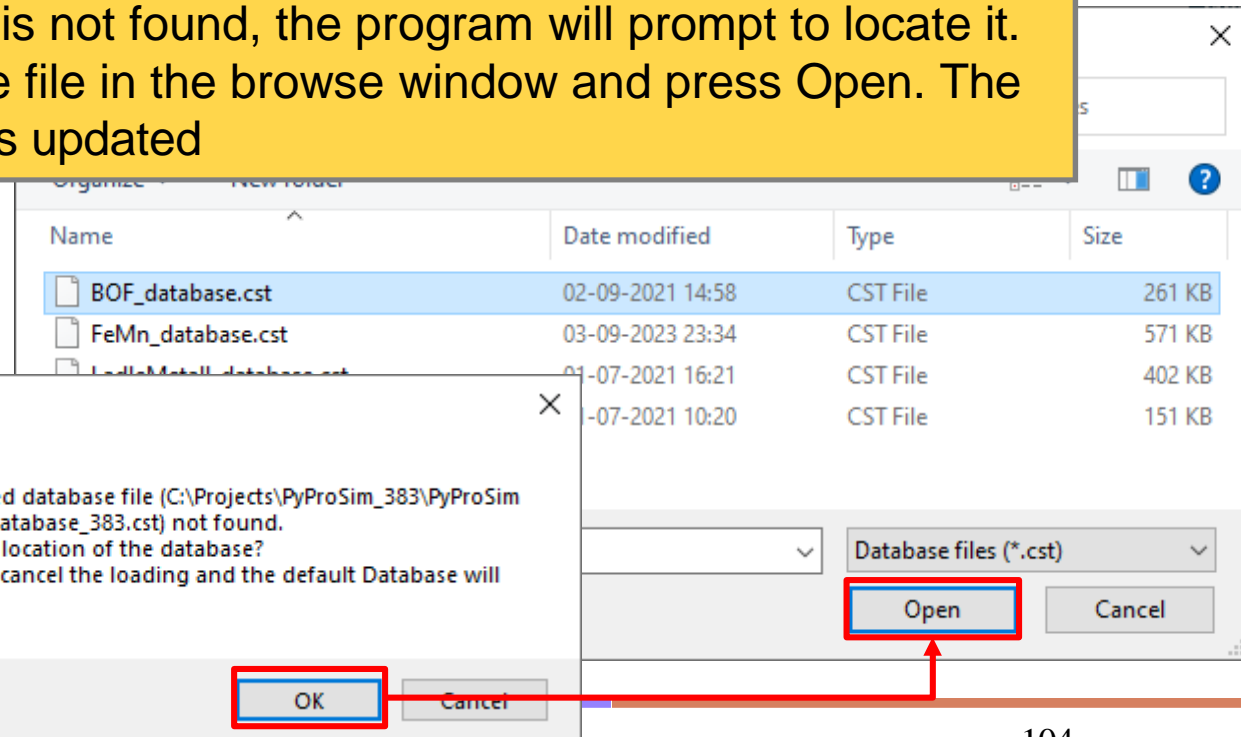
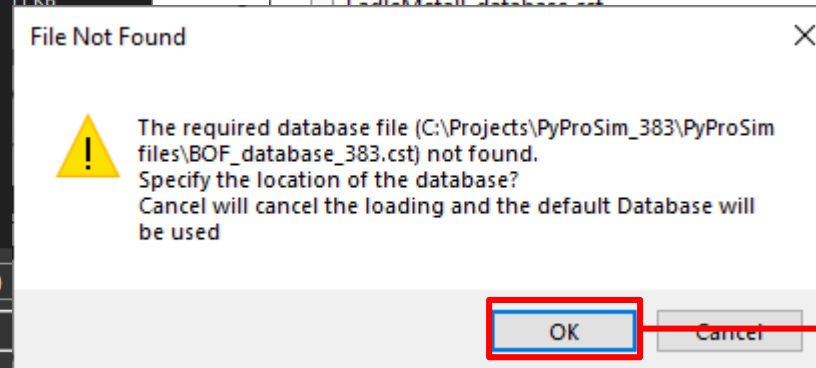
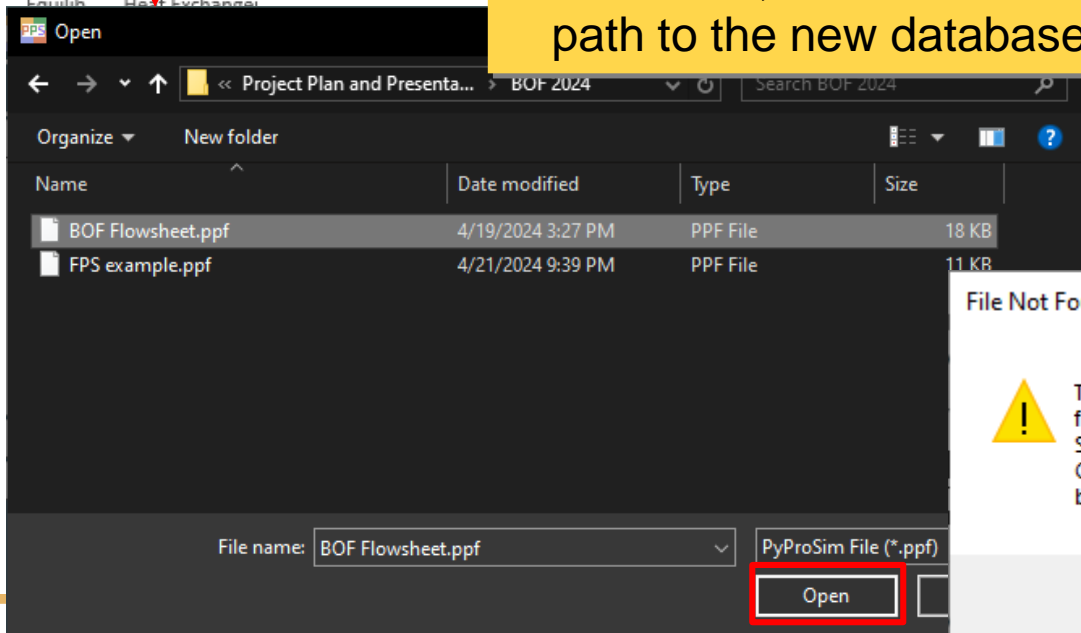
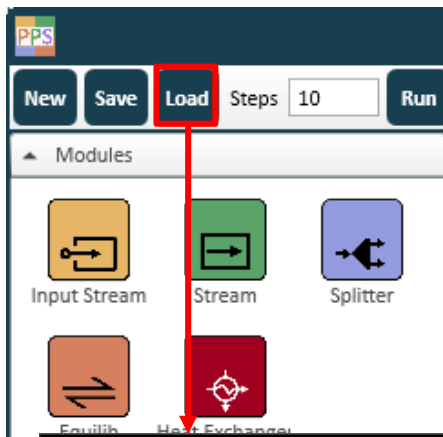
Save the flowsheet



- Press the button Save in the toolbar to save the current flowsheet. In the browse window, select the location and enter the name of the flowsheet. The flowsheet information are saved in ppf format (encrypted)
- Along with all the modules data, the path to the selected database file (*.cst) and Excel Files (if Excel Links are used in the modules) are stored in the ppf file

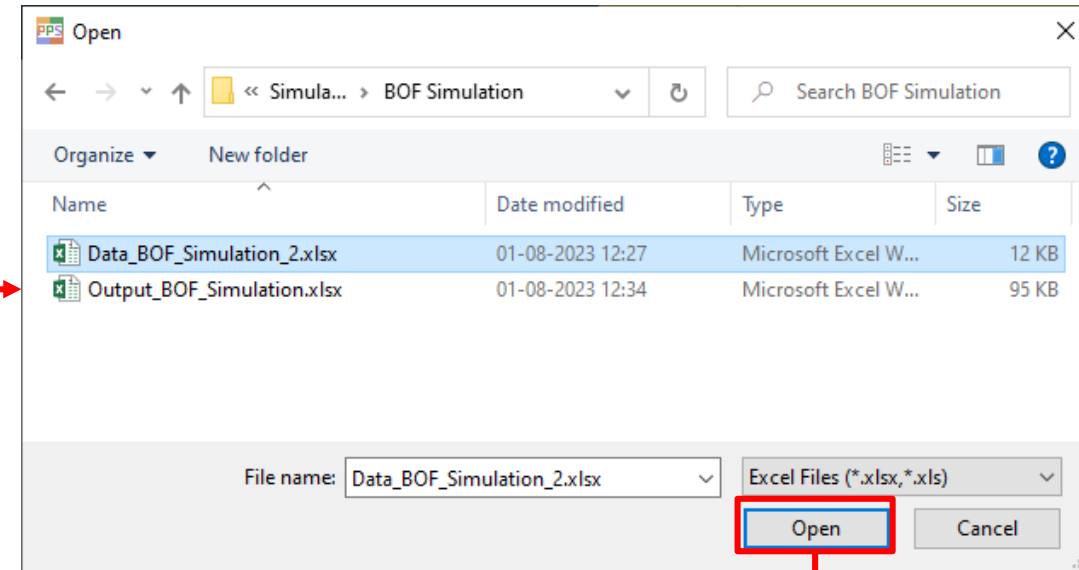
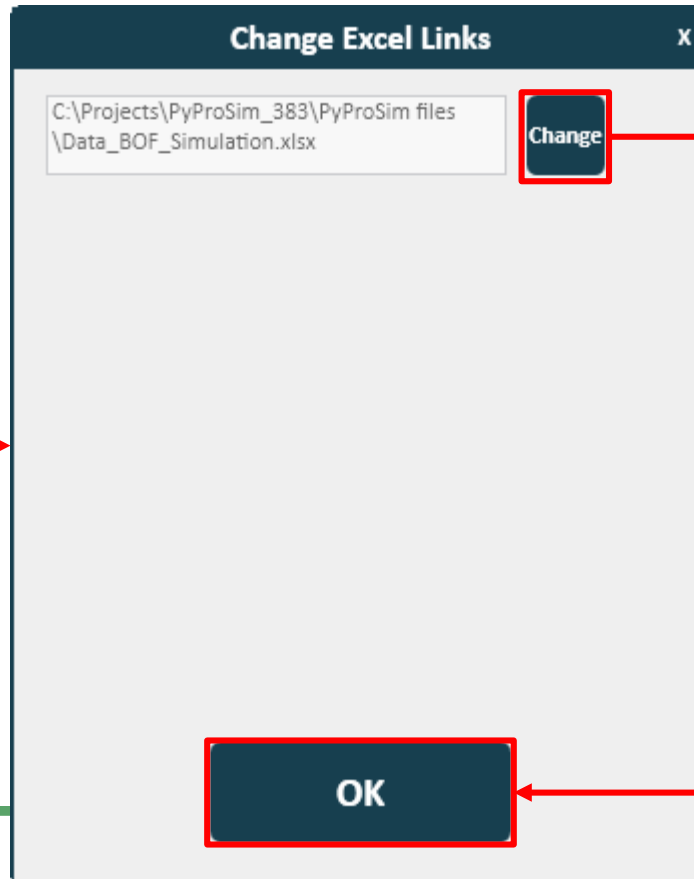
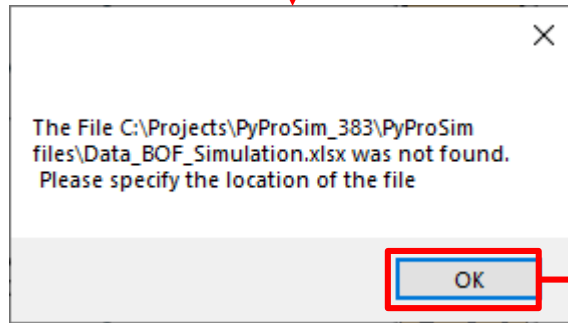
Load an existing flowsheet

- Press the button Load in the toolbar to open an existing flowsheet. In the browse window, select the flowsheet to open (in ppf format) **⚠ The current flowsheet will be lost if not saved!**
- Each flowsheet is connected to a database file (*.cst) and Excel Files (if Excel Links are used in the modules). These files must exist at the specified path for the program to load the data correctly
- If the connected database file is not found, the program will prompt to locate it. Press OK, locate the database file in the browse window and press Open. The path to the new database file is updated



Load an existing flowsheet (continued)

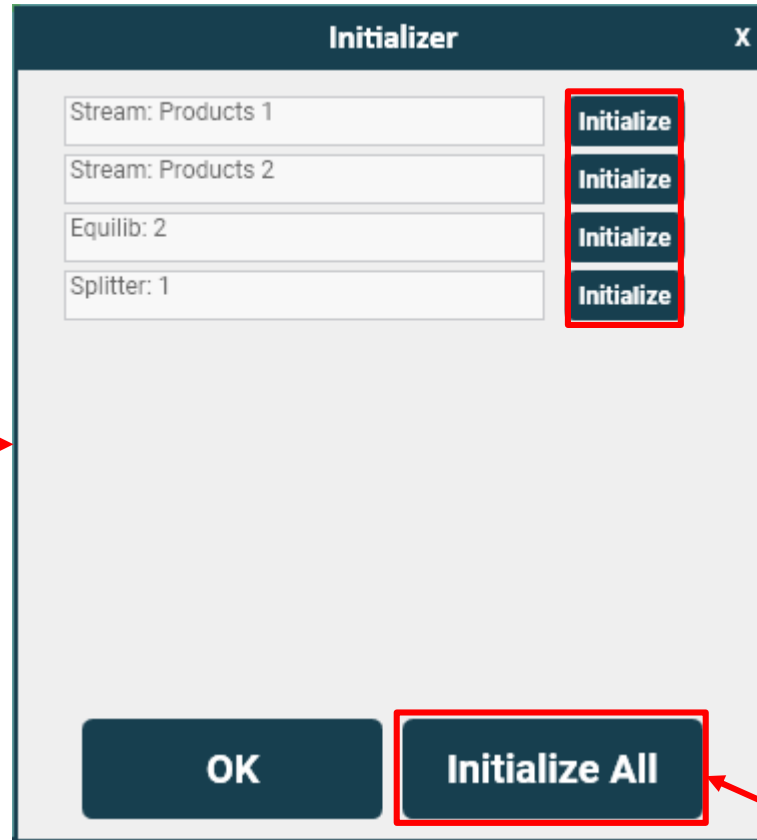
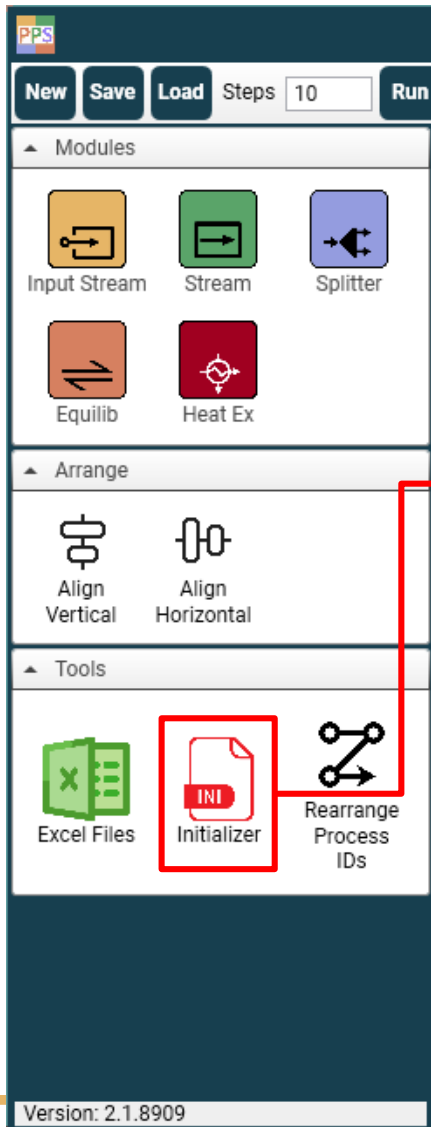
- Similarly, if the connected Excel file(s) is not found, the program will prompt to locate the File(s). After pressing OK, the Excel File tool will open automatically. Press the button Change next to the Excel File path. In the browse window, locate the Excel file and press Open. The path to the new Excel file is now updated. Press OK to close the Excel File tool



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 - Align the process modules in the flowsheet
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- **Step 3: Check the modules – The Initializer**
- Step 4: Run the process flowsheet
- Step 5: View the Results (Output Excel File)

Step 3: Check the modules – The Initializer



The initializer is a function in the Local Controls panel that checks in each module if all the necessary information has been entered by the user. The modules that are not entirely initialized are listed in the Initializer window. Click on the Initialize button next to each listed module to open it and make changes where needed.

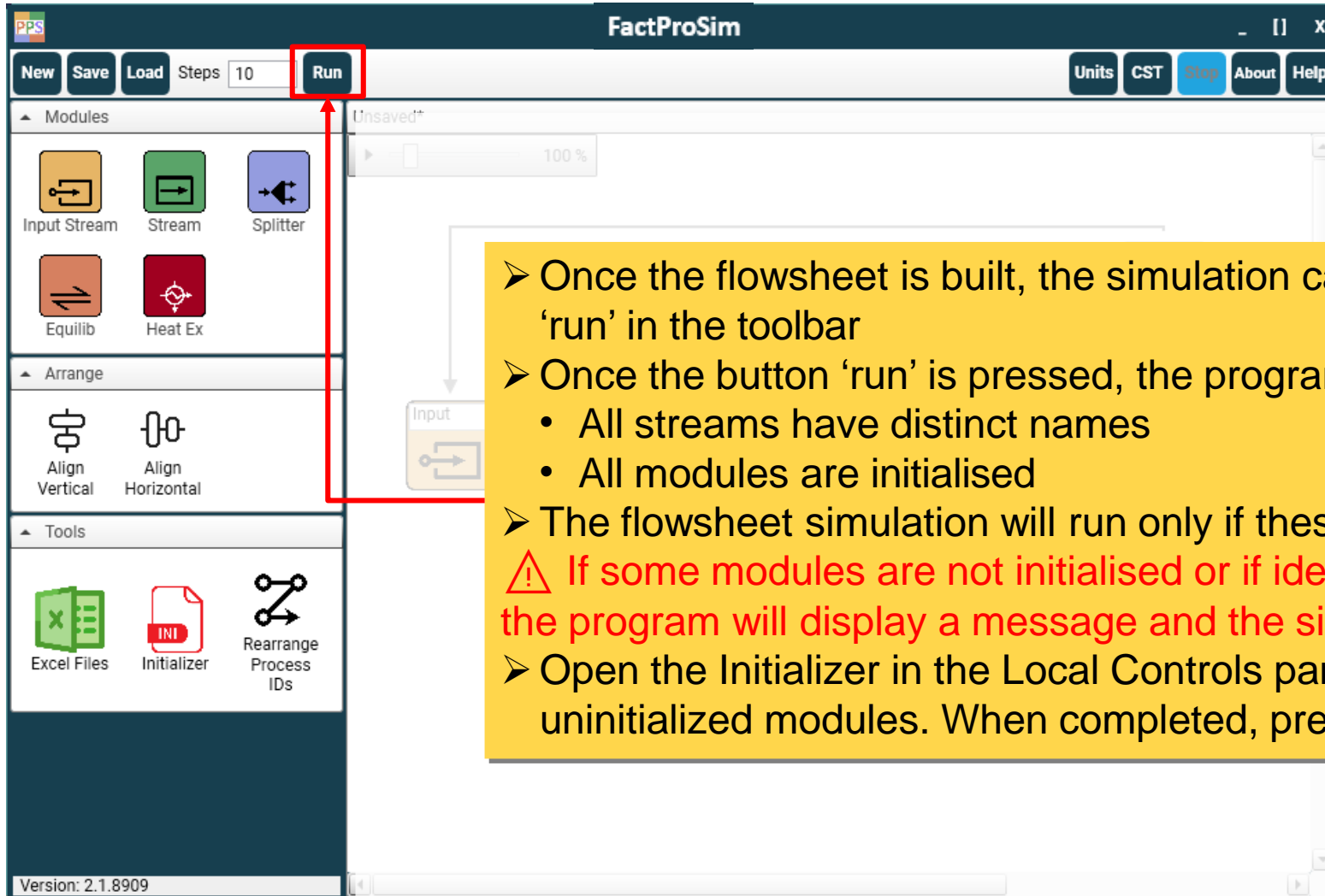
⚠ Rearranging, adding or removing modules and connections in the flowsheet, changing phase selection or adding new elements can cause the connected initialized modules to become uninitialized

💡 Sometimes no changes are needed in the uninitialized module. However, the user must still open and check each module listed in the Initializer window. Alternatively, user can automate the initialization process by clicking on “Initialize All” button. Press the OK button in the module to reinitialize it.

Description of the program

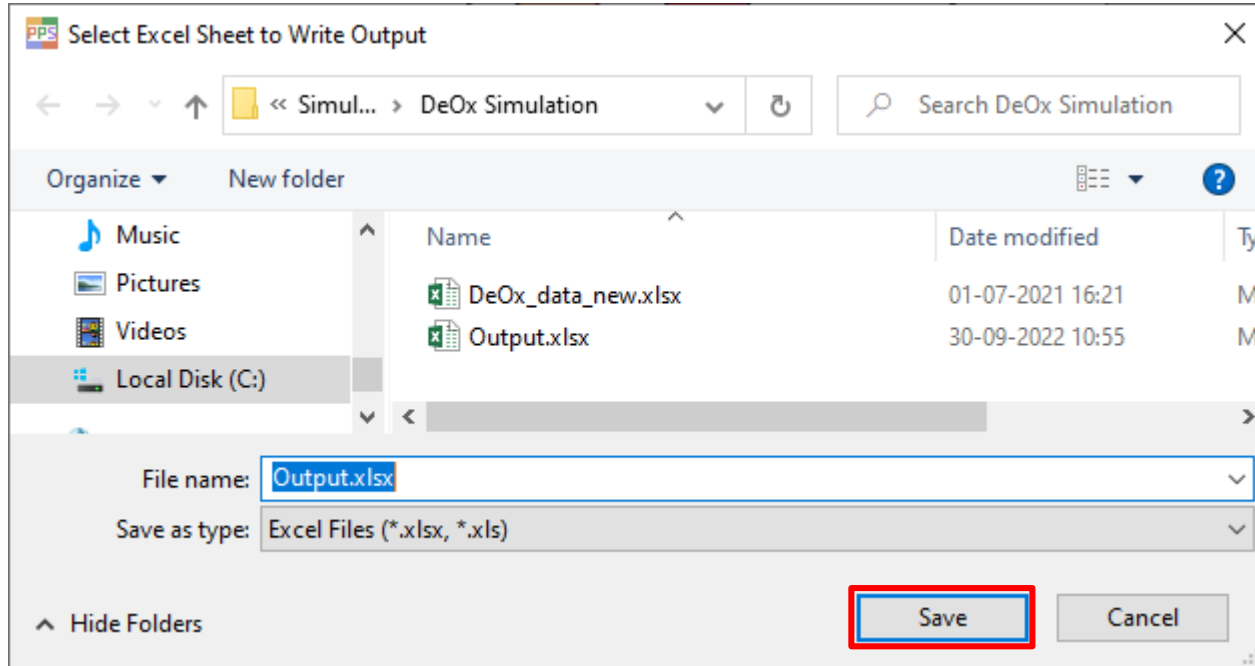
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Step 4: Run the process flowsheet



- Once the flowsheet is built, the simulation can be started by clicking the button 'run' in the toolbar
- Once the button 'run' is pressed, the program first do several checks:
 - All streams have distinct names
 - All modules are initialised
- The flowsheet simulation will run only if these checks return no errors.
⚠ If some modules are not initialised or if identical stream names are found, the program will display a message and the simulation is aborted.
- Open the Initializer in the Local Controls panel to view and open the uninitialized modules. When completed, press the button 'run' again

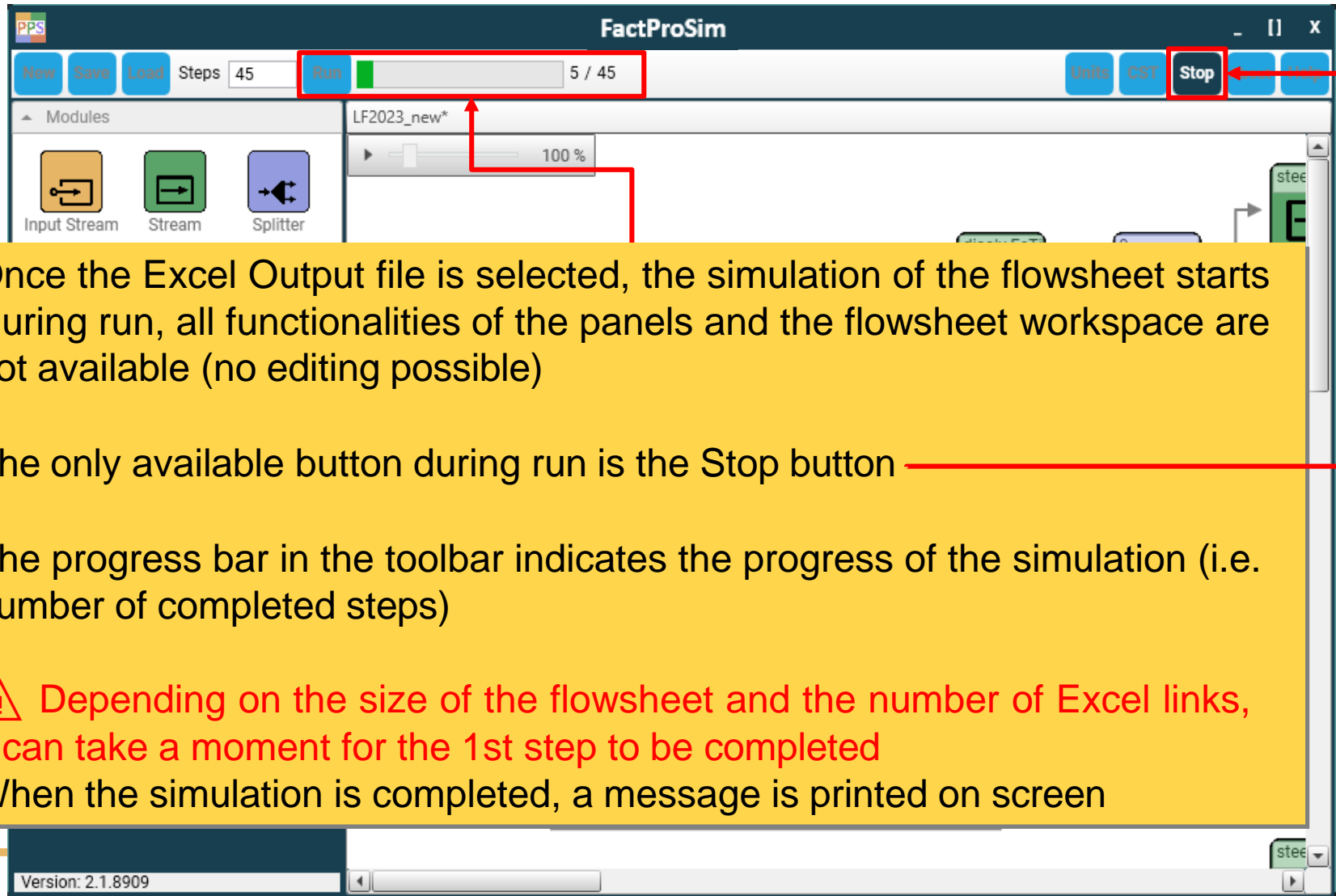
Run the process flowsheet



- If no errors are found, the program will prompt for an Excel output file (default Output.xlsx) where the simulation results will be printed
- A new Excel file can be created or an existing Excel file can be selected

⚠ When selecting an existing Excel file, previous calculation results will be overwritten in the worksheets matching the names of the streams in the current flowsheet. Other worksheets in the existing Excel file will not be erased or modified

Run the process flowsheet



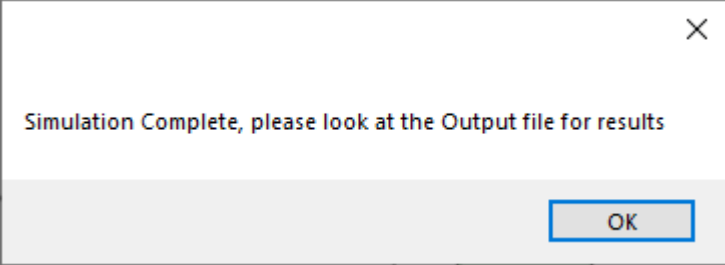
Once the Excel Output file is selected, the simulation of the flowsheet starts. During run, all functionalities of the panels and the flowsheet workspace are not available (no editing possible).

The only available button during run is the Stop button.

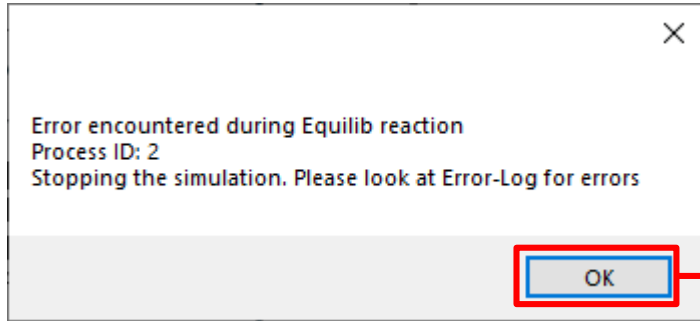
The progress bar in the toolbar indicates the progress of the simulation (i.e. number of completed steps).

⚠ Depending on the size of the flowsheet and the number of Excel links, it can take a moment for the 1st step to be completed.

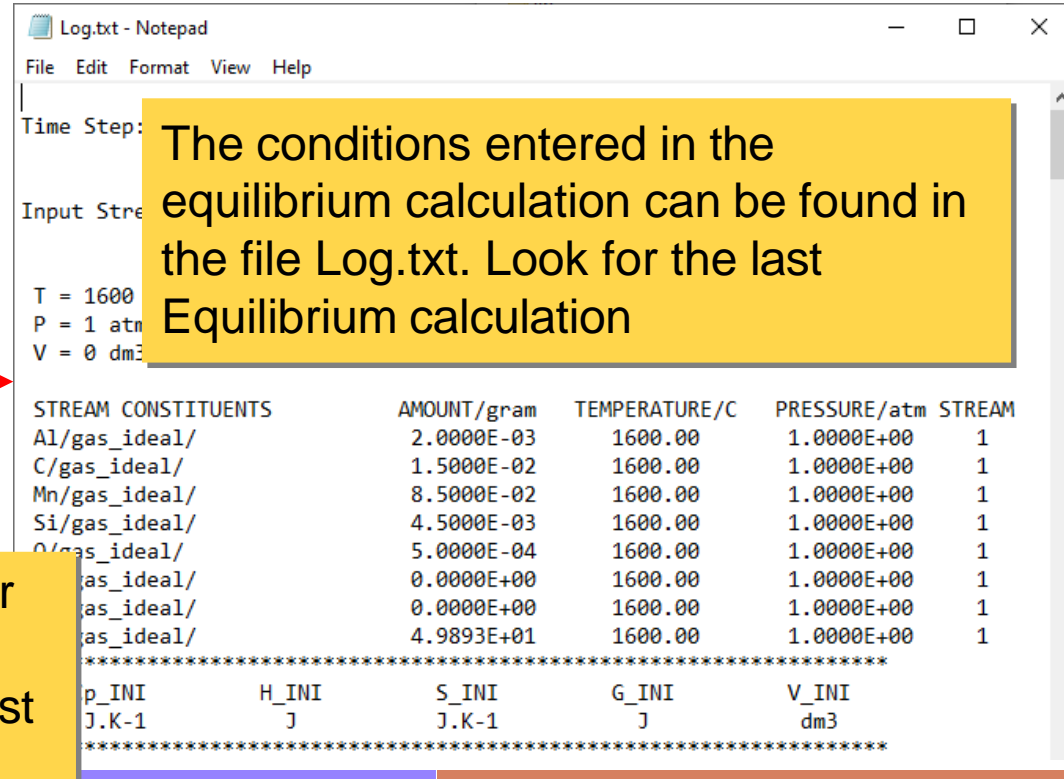
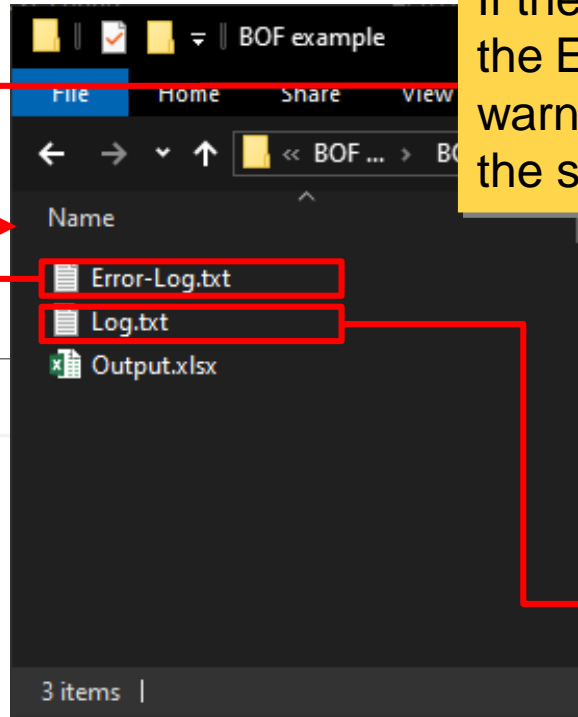
When the simulation is completed, a message is printed on screen.



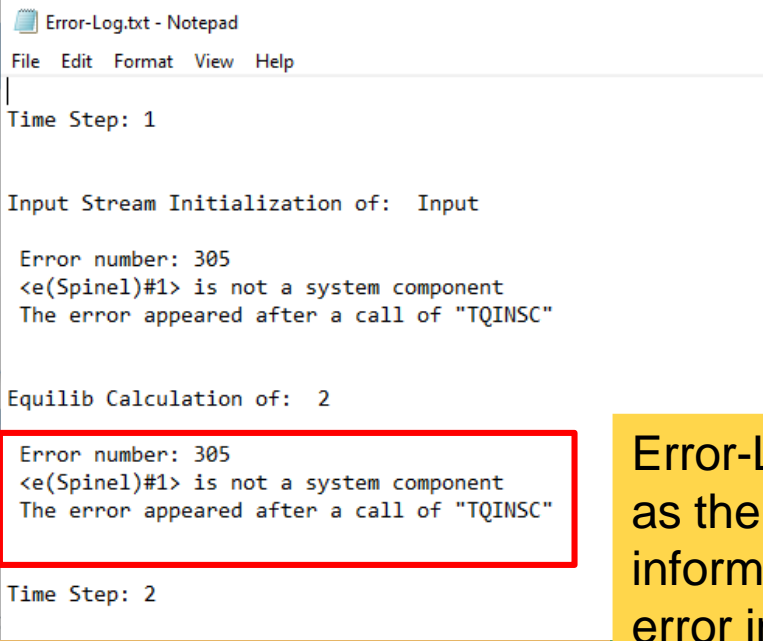
Error during run



If the program encountered an error during the Equilibrium calculation, the program will warn the user with a message box and stop the simulation



The conditions entered in the equilibrium calculation can be found in the file Log.txt. Look for the last Equilibrium calculation



Error-Log.txt, located in the same folder as the output file (Output.xlsx), gives information on the error. Look for the last error in the file

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- **Step 5: View the Results (Output Excel File)**

Step 5: View the results – Excel Output file

Output2.xlsx - Excel

File Home Insert Page Layout Formulas Data Review View Help Tell me what you want to do Share

Clipboard Font Alignment Number Styles Cells Editing

N20

	A	B	C	D	E	F	G	H	I	J	
1		Reaction: 2									
2	Time	Temperature [C]	DELTA Cp [J.K-1]	DELTA H [J]	DELTA S [J.K-1]	DELTA G [J]	DELTA V [dm3]				
3	1	1500	-13.5391594	265499.8601	85.72284892	120779.0093	104.2216861				
4	2	1500	3.00021E-08	-0.00433197	-1.39163E-06	-0.0018644	-1.73285E-06				
5	3	1500	3.87014E-08	3.31013E-13	1.97796E-16	-1.97086E-14	4.26708E-16				
6	4	1500	3.09611E-08	2.65079E-13	1.58388E-16	-1.57673E-14	3.41404E-16				
7	5	1500	2.47689E-08	2.12066E-13	1.26712E-16	-1.26135E-14	2.73024E-16				
8	6	1500	1.98151E-08	1.69522E-13	1.01295E-16	-1.0091E-14	2.18475E-16				
9	7	1500	1.58521E-08	1.35657E-13	8.10591E-17	-8.07282E-15	1.7478E-16				
10	8	1500	1.26817E-08	1.086E-13	6.48893E-17	-6.45805E-15	1.39809E-16				
11	9	1500	1.01453E-08	8.67284E-14	5.18256E-17	-5.16636E-15	1.11831E-16				
12	10	1500	8.11626E-09	6.95267E-14	4.15418E-17	-4.13319E-15	8.94551E-17				
13											
14											
15											
16											

Reaction Information Output 1 Output 2

Ready

The results in the Excel output file are organised in several worksheets:

1. The worksheet Reaction Information provides a summary of the equilibrium calculation for each Equilib module at each step

View the results – Excel Output file (continued)

The screenshot shows an Excel spreadsheet titled 'Output2.xlsx'. The active worksheet is 'Products 1', which is circled in red. The spreadsheet displays simulation results for a 'Fe-liq' stream. The columns represent various chemical species and their concentrations in g/g. The rows represent different steps in the process, with columns for Time, Temperature, and Amount of each species.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	
1			Fe-liq																			
2	Time	Temperatu	Amount (ç	Fe (g/g)	Al (g/g)	C (g/g)	Ca (g/g)	Mn (g/g)	O (g/g)	Si (g/g)	Mg (g/g)	MgO (g/g)	CaO (g/g)	AlO (g/g)	SiO (g/g)	MnO (g/g)	Al2O (g/g)	Fe (g/g)	Mn (g/g)	Ca (g/g)	Si (g/g)	Al (ç
3	1	1600	40	0.99786	3.87E-05	0.0003	0	0.0017	9.14E-06	9E-05	0	0	0	2.11E-06	4.55E-09	2.67E-07	2.7E-08	0.99786	0.0017	0	9E-05	
4	2	1500	31.99972	0.997869	3.45E-05	0.0003	0	0.0017	5.34E-06	9E-05	0	0	0	1.64E-06	2.66E-09	1.68E-07	2.42E-08	0.997869	0.0017	0	9E-05	3.8
5	3	1500	25.59978	0.997869	3.45E-05	0.0003	0	0.0017	5.34E-06	9E-05	0	0	0	1.64E-06	2.66E-09	1.68E-07	2.42E-08	0.997869	0.0017	0	9E-05	3.8
6	4	1500	20.47982	0.997869	3.45E-05	0.0003	0	0.0017	5.34E-06	9E-05	0	0	0	1.64E-06	2.66E-09	1.68E-07	2.42E-08	0.997869	0.0017	0	9E-05	3.8
7	5	1500	16.38386	0.997869	3.45E-05	0.0003	0	0.0017	5.34E-06	9E-05	0	0	0	1.64E-06	2.66E-09	1.68E-07	2.42E-08	0.997869	0.0017	0	9E-05	3.8
8	6	1500	13.10709	0.997869	3.45E-05	0.0003	0	0.0017	5.34E-06	9E-05	0	0	0	1.64E-06	2.66E-09	1.68E-07	2.42E-08	0.997869	0.0017	0	9E-05	3.8
9	7	1500	10.48567	0.997869	3.45E-05	0.0003	0	0.0017	5.34E-06	9E-05	0	0	0	1.64E-06	2.66E-09	1.68E-07	2.42E-08	0.997869	0.0017	0	9E-05	3.8
10	8	1500	8.388535	0.997869	3.45E-05	0.0003	0	0.0017	5.34E-06	9E-05	0	0	0	1.64E-06	2.66E-09	1.68E-07	2.42E-08	0.997869	0.0017	0	9E-05	3.8
11	9	1500	6.710828	0.997869	3.45E-05	0.0003	0	0.0017	5.34E-06	9E-05	0	0	0	1.64E-06	2.66E-09	1.68E-07	2.42E-08	0.997869	0.0017	0	9E-05	3.8
12	10	1500	5.368663	0.997869	3.45E-05	0.0003	0	0.0017	5.34E-06	9E-05	0	0	0	1.64E-06	2.66E-09	1.68E-07	2.42E-08	0.997869	0.0017	0	9E-05	3.8
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2. The other worksheets correspond to each Stream module in the flowsheet (the worksheet being named after the Stream). Each worksheet contains, for each step, the calculated temperature and amount of each phase in the Stream, and composition of gas and solution phases if selected (both species and elemental)