ENGINEERING
COLLEGE OF ENGINEERING
SEOUL NATIONAL UNIVERSITY
서 울 대 학 교 공 과 대 학

Department of Materials Science and Engineering

FactProSim

Installation Guide and Program Description
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Content

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

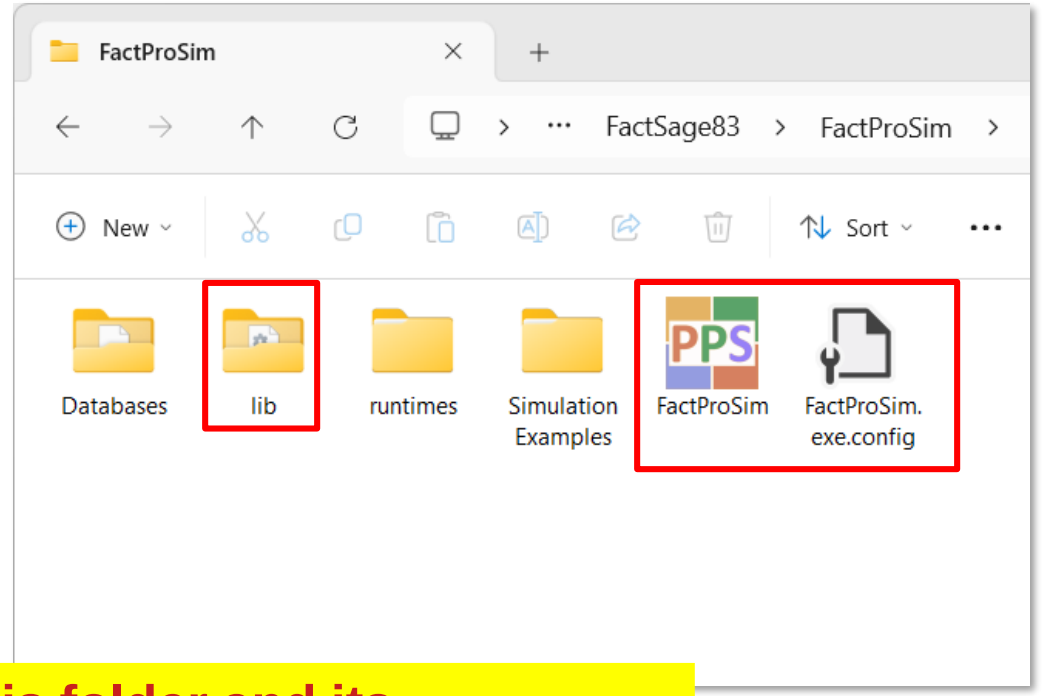
To install FactProSim on your Windows computer,

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

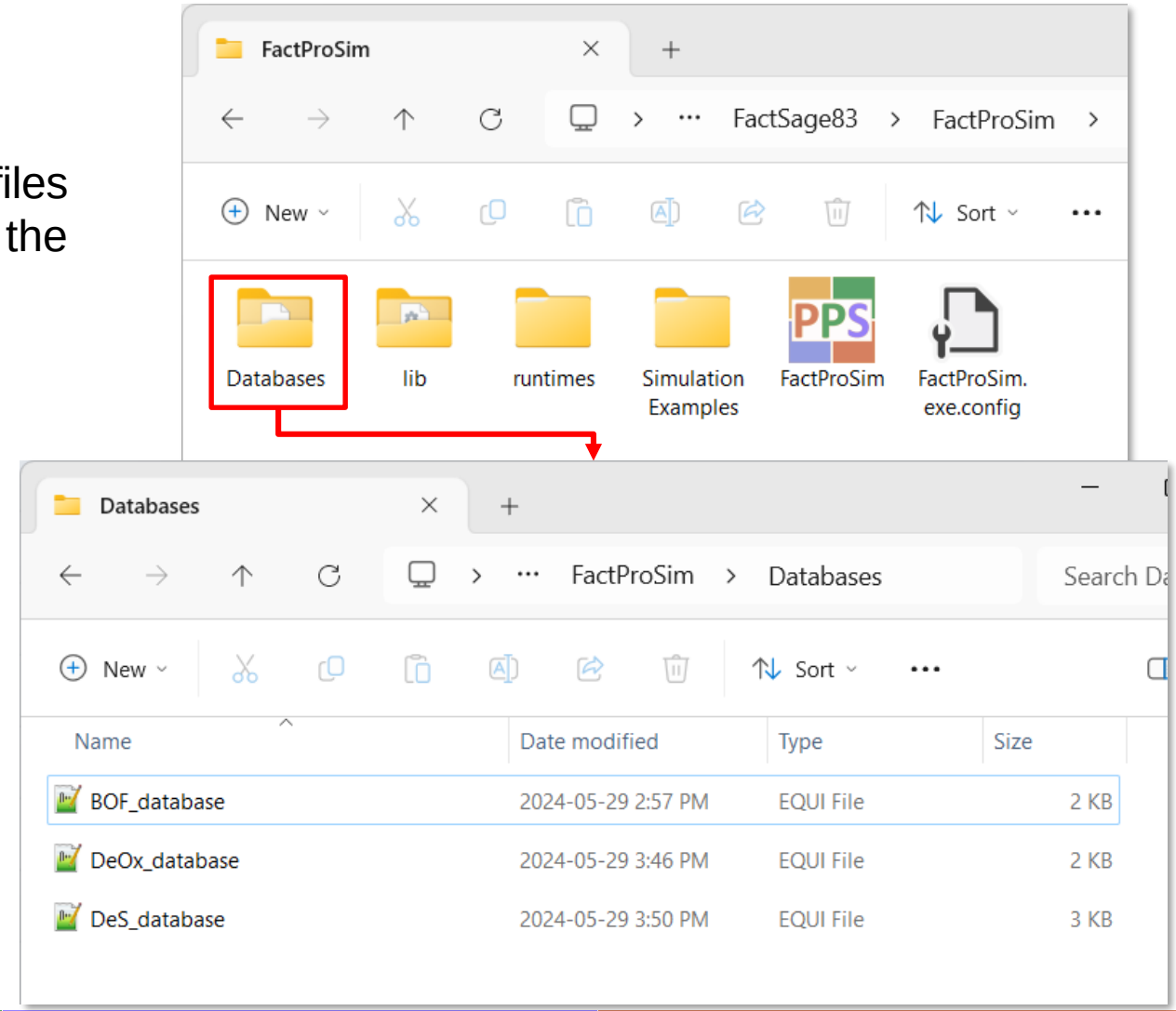


⚠ **Do not rename, move or delete these files, this folder and its content! These 3 items are required for the program to run**
The folder *lib* AND the file *FactProSim.exe.config* MUST be located in the same folder as *FactProSim.exe*. If not, the program FactProSim won't run

Overview of the FactProSim package

The FactProSim package contains (continued):

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

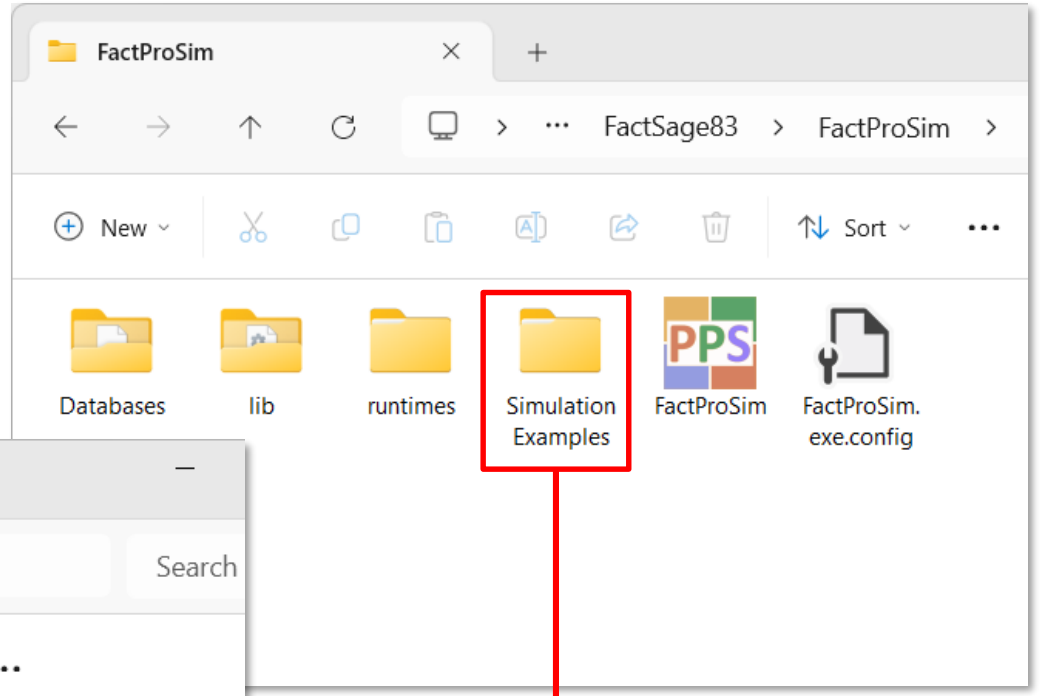


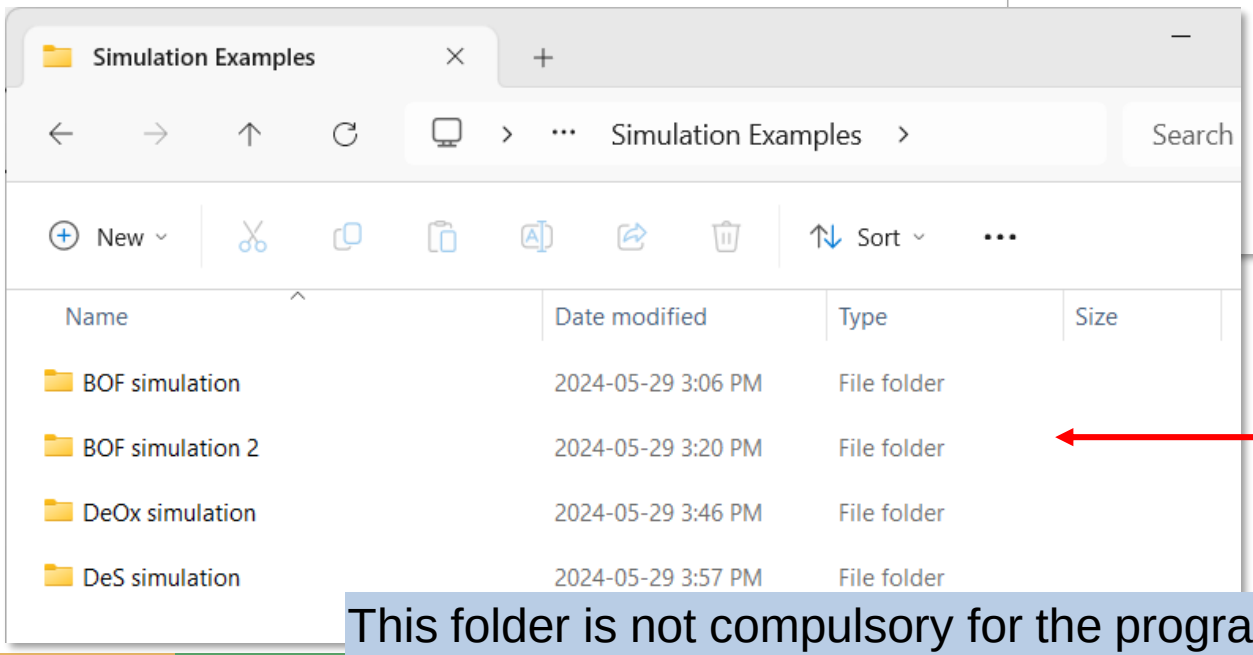
This folder is not compulsory for the program FactProSim to run. It can be modified, moved or deleted by the user

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





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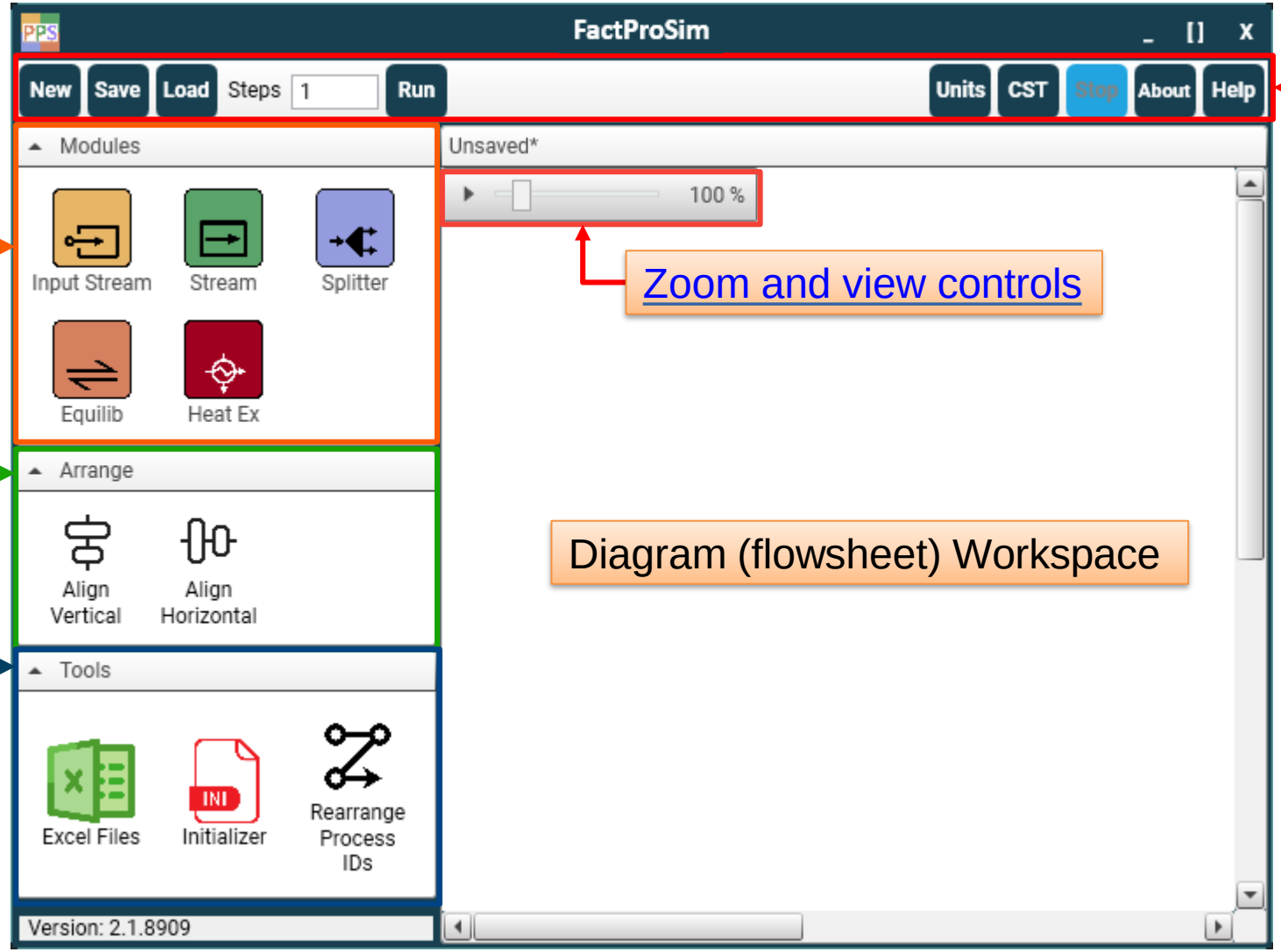
Description of the program

Overview of the Main Window



Toolbar

Modules Panel

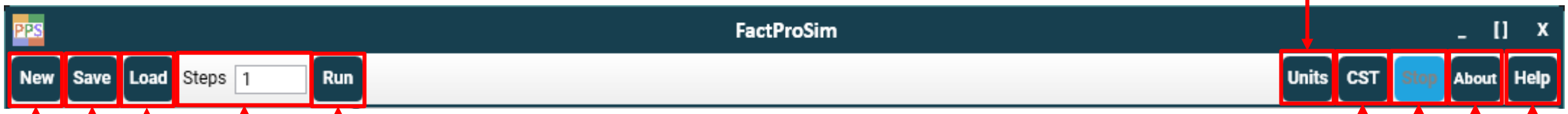
Zoom and view controls

Arrange Panel

Diagram (flowsheet) Workspace

Extra Tools

Commands in the Toolbar



Units

Run the simulation

Load a database file (*.cst)

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

Abort the simulation (activated during run)

Load an existing diagram (ppf, encrypted)

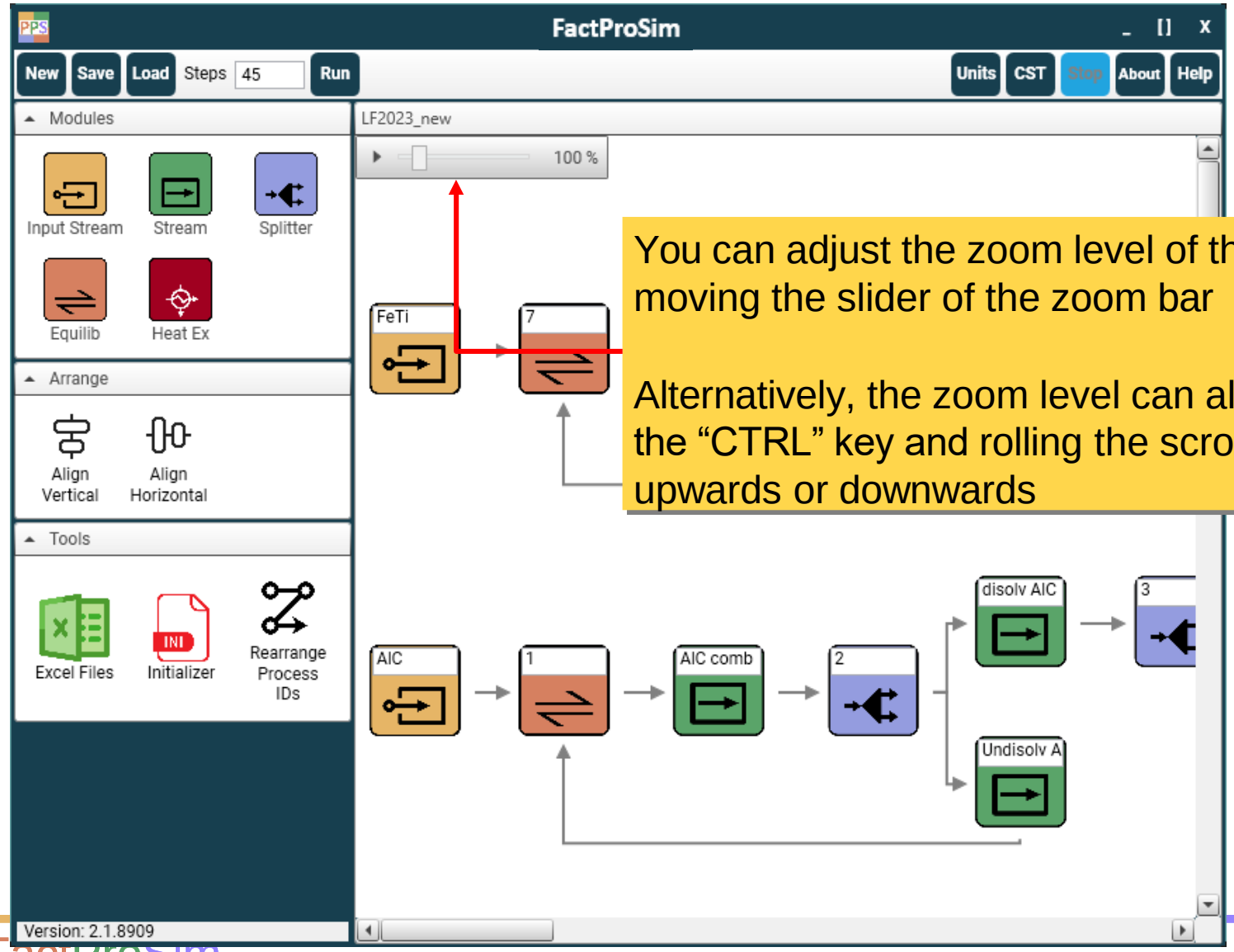
Display developers names And contact information

Save the current diagram (ppf, encrypted)

Open the user manual for FactProSim

Create a new blank diagram
⚠ The current diagram will be lost if unsaved

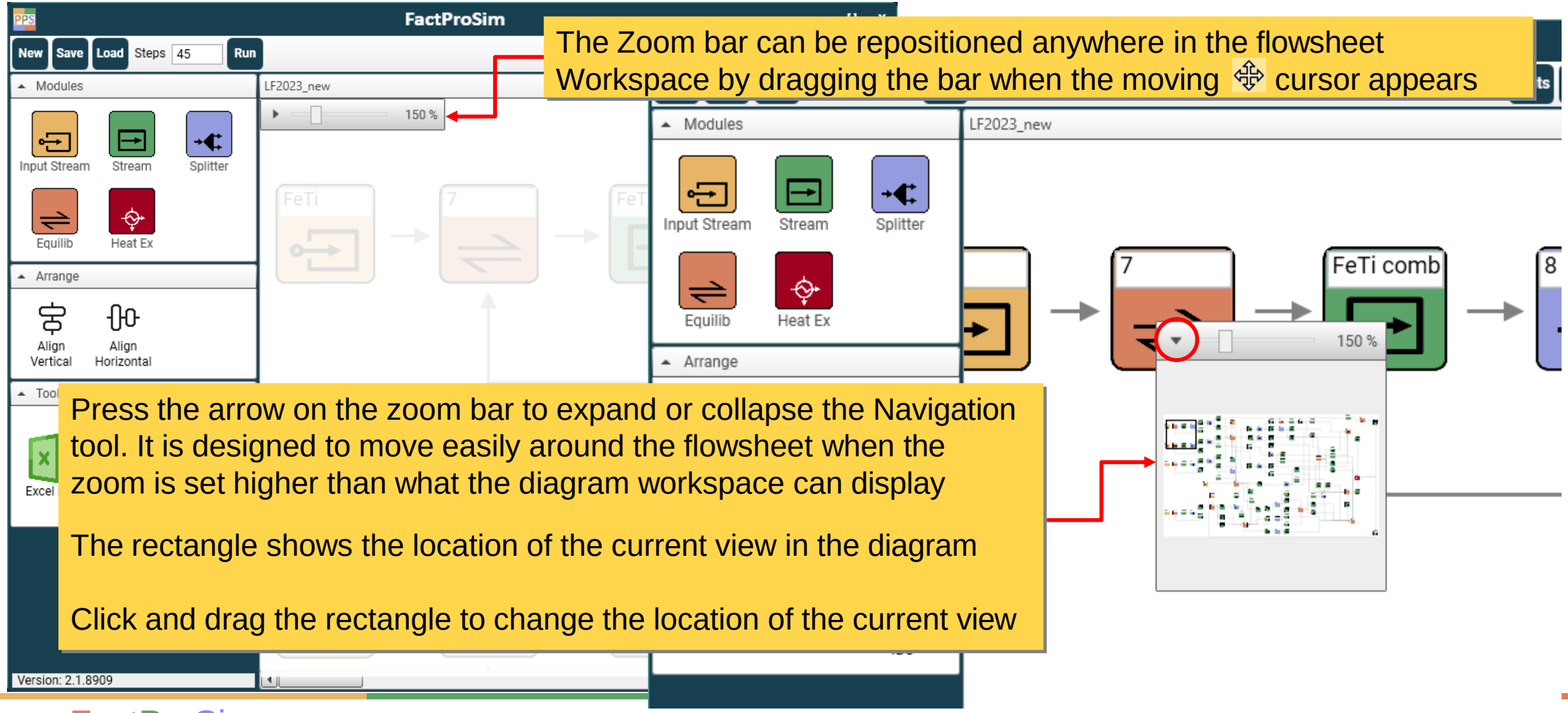
Zoom and view controls



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)



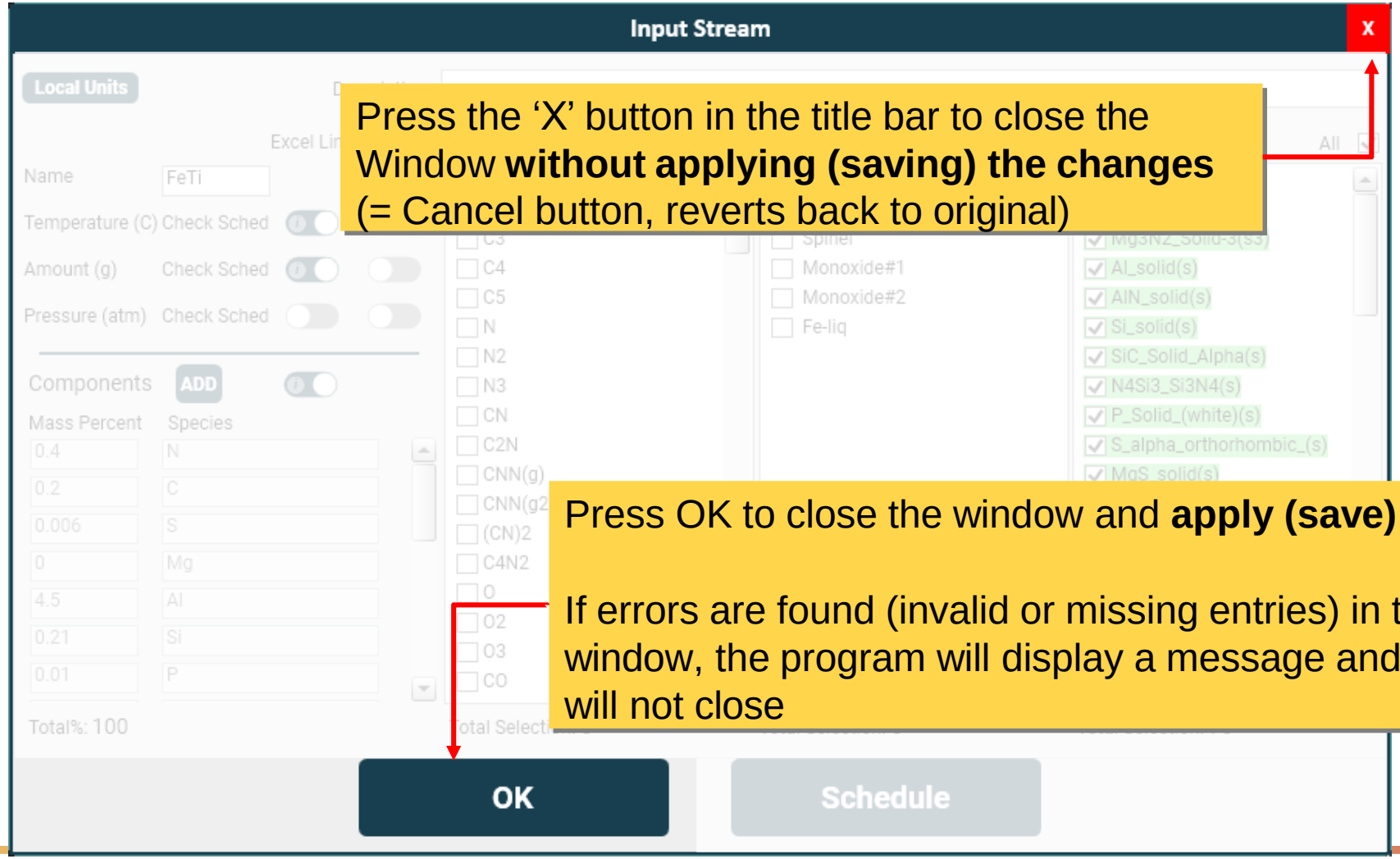
The Zoom bar can be repositioned anywhere in the flowsheet Workspace by dragging the bar when the moving cursor appears

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

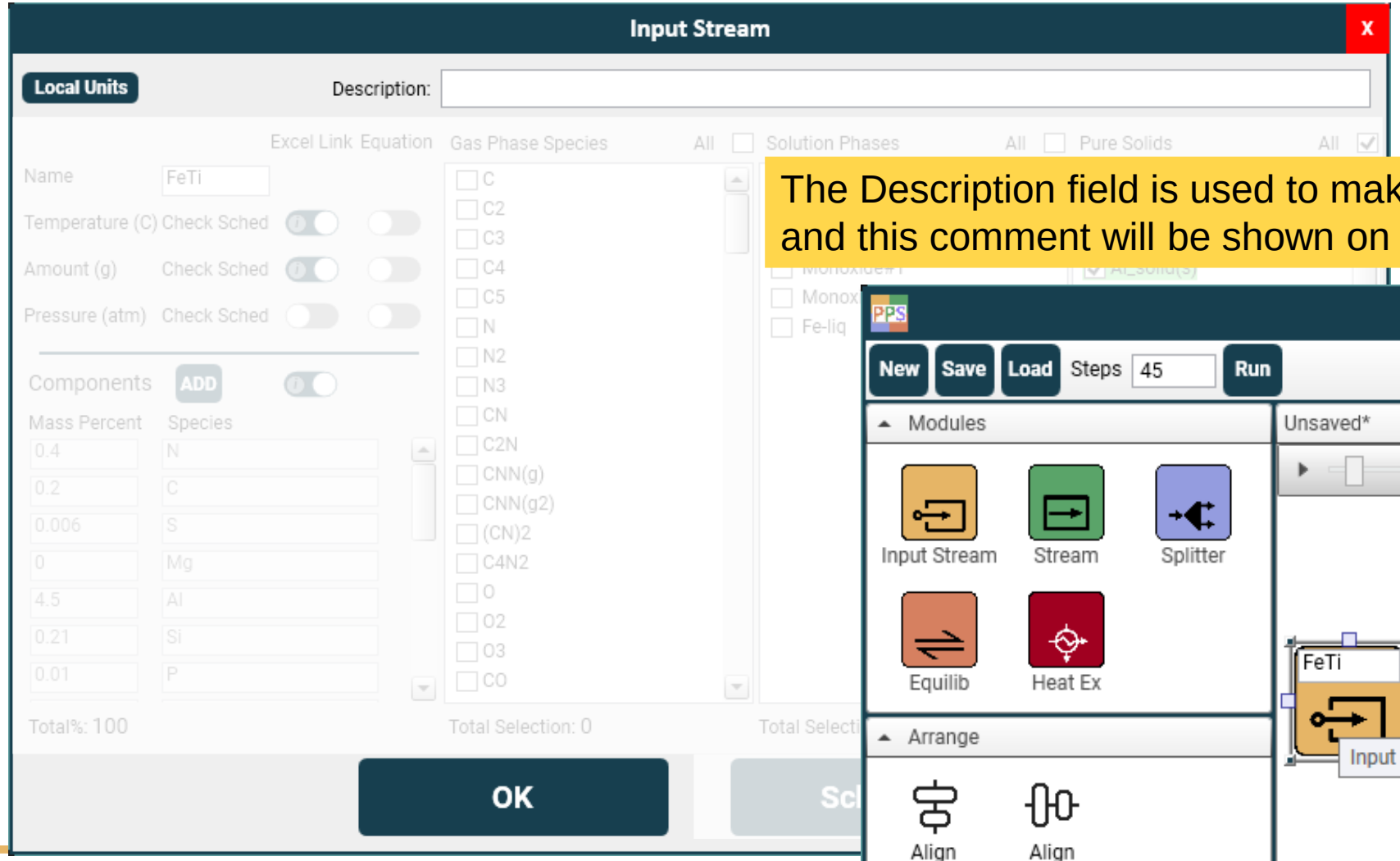


Press the ‘X’ button in the title bar to close the Window **without applying (saving) the changes** (= Cancel button, reverts back to original)

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

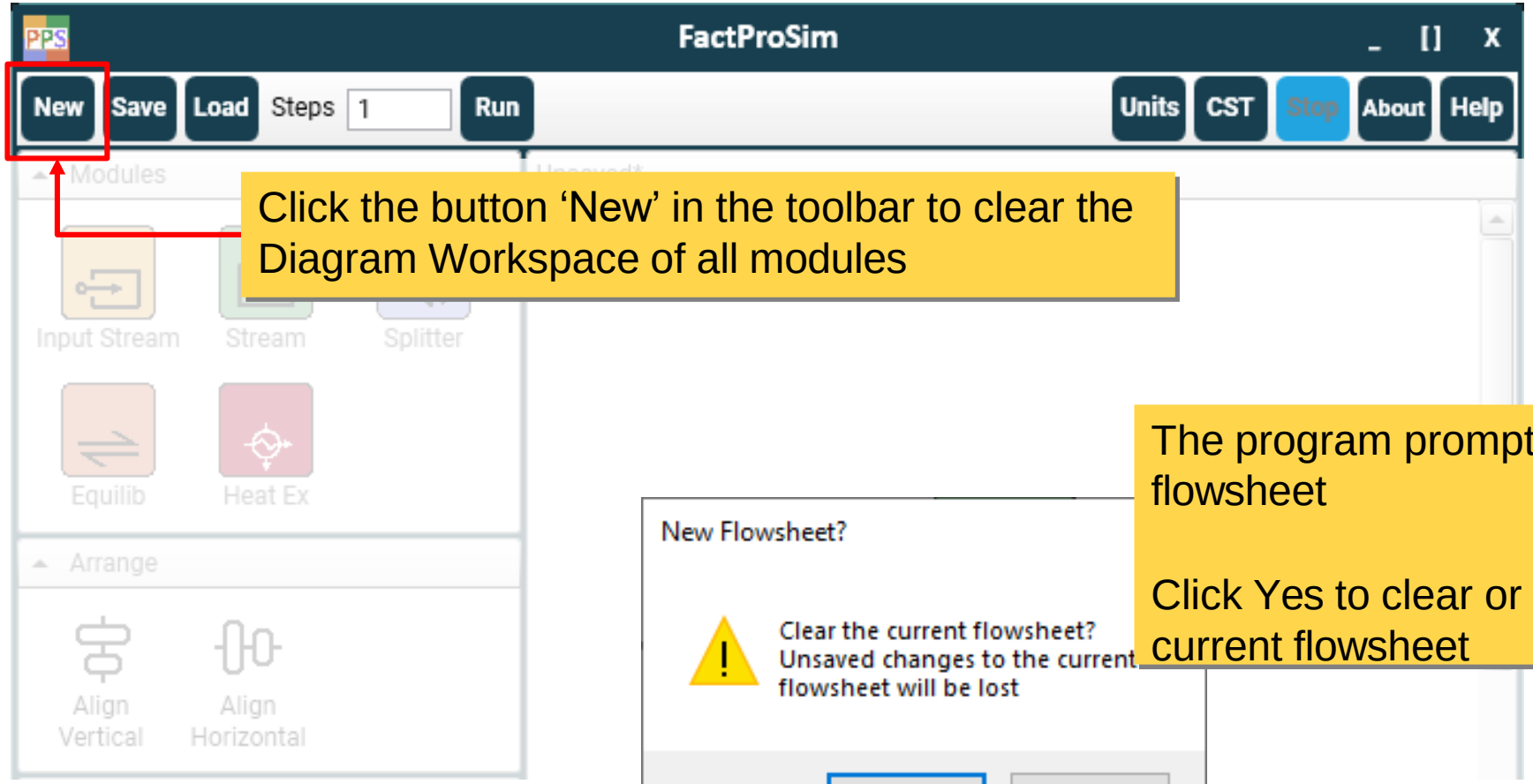
General behavior in windows



The Description field is used to make comments about the window and this comment will be shown on the flowsheet outside

Working on flowsheets

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



The program prompts to clear the current flowsheet

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

- 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)

Step 1: Create a database file

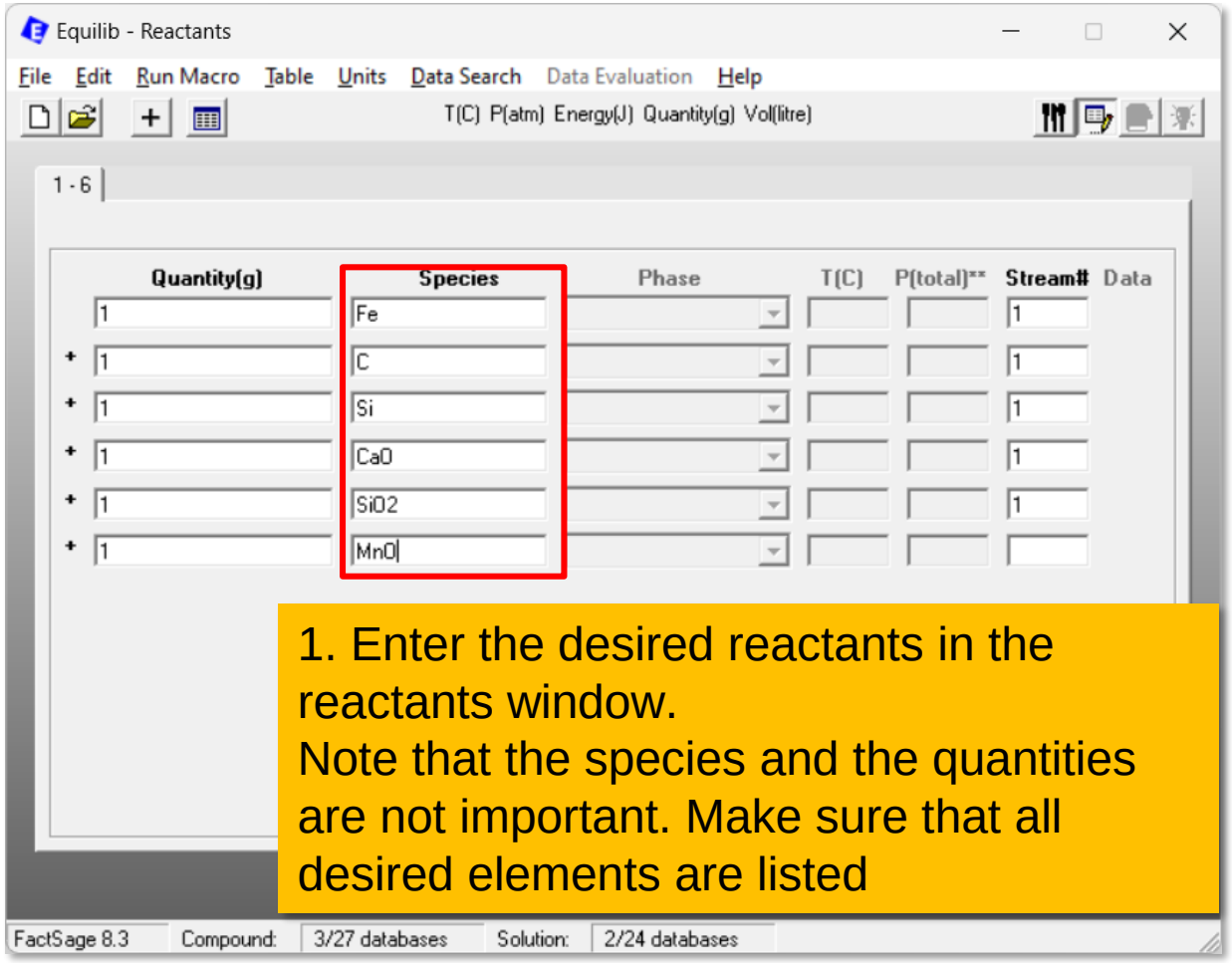
FactProSim utilizes ‘transparent’ ChemSage file (*.cst file), which is a thermochemical data file to store the thermodynamic properties of the phases to be included in the flowsheet. In other words, these cst files are a subset of the large commercial and private databases included in FactSage

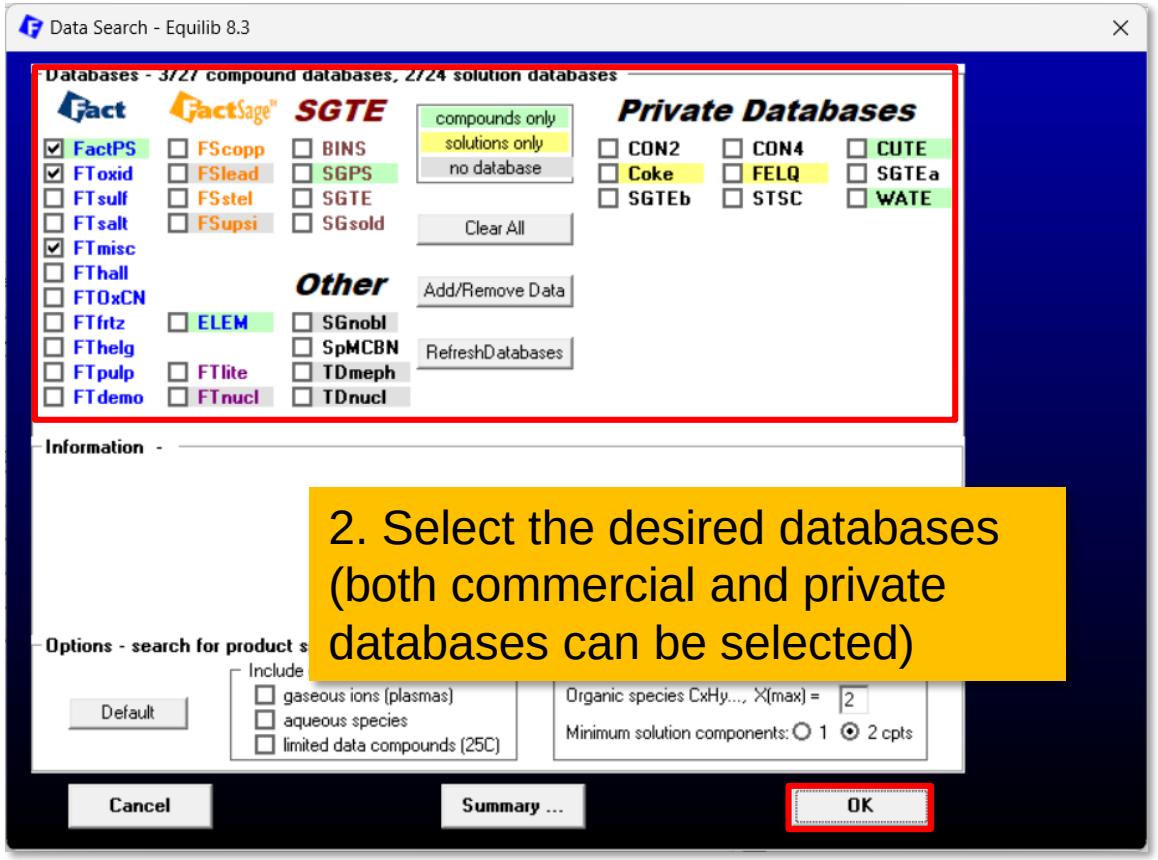
These thermochemical data cst files can be created with the Equilib module of FactSage, either

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

Step 1: Create a database file

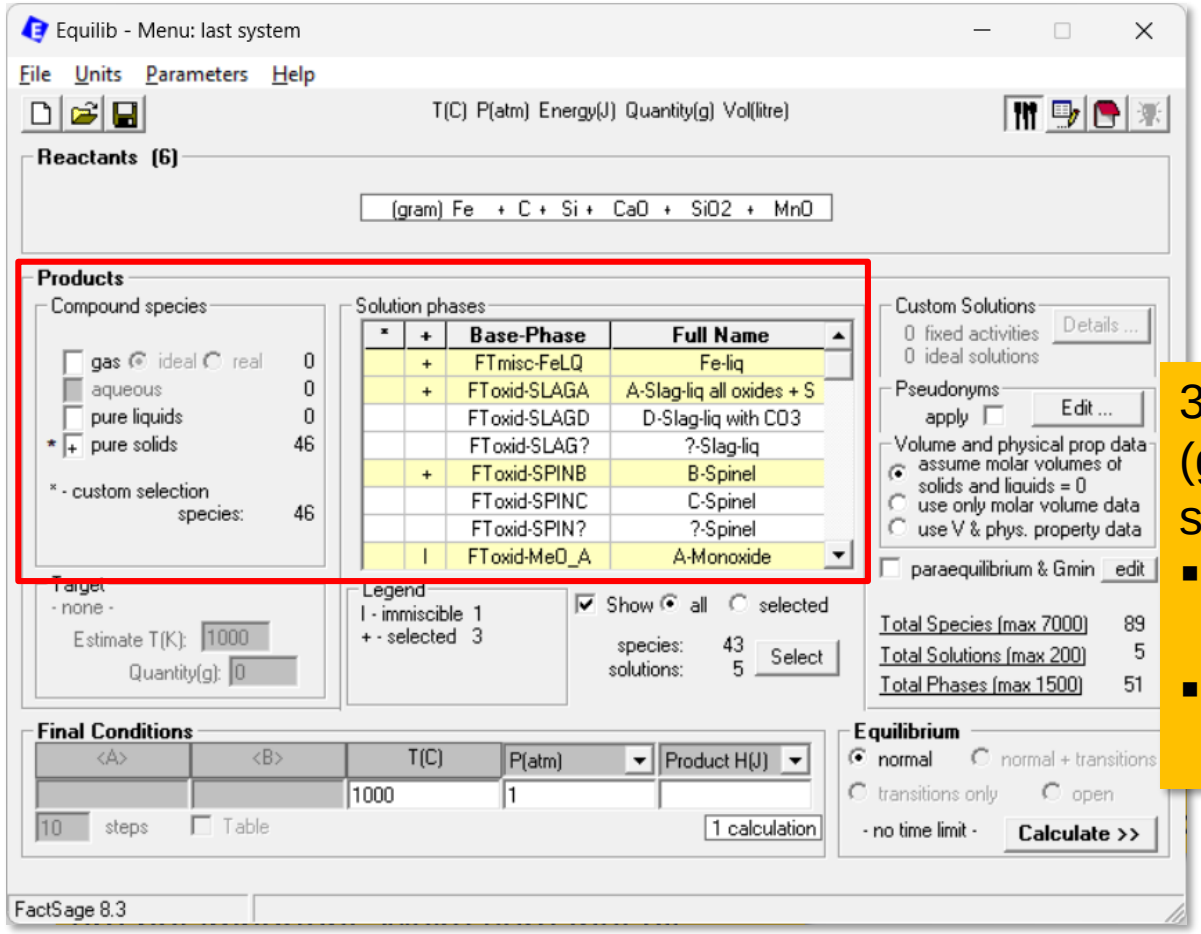
- From reactants and phase selection





Step 1: Create a database file

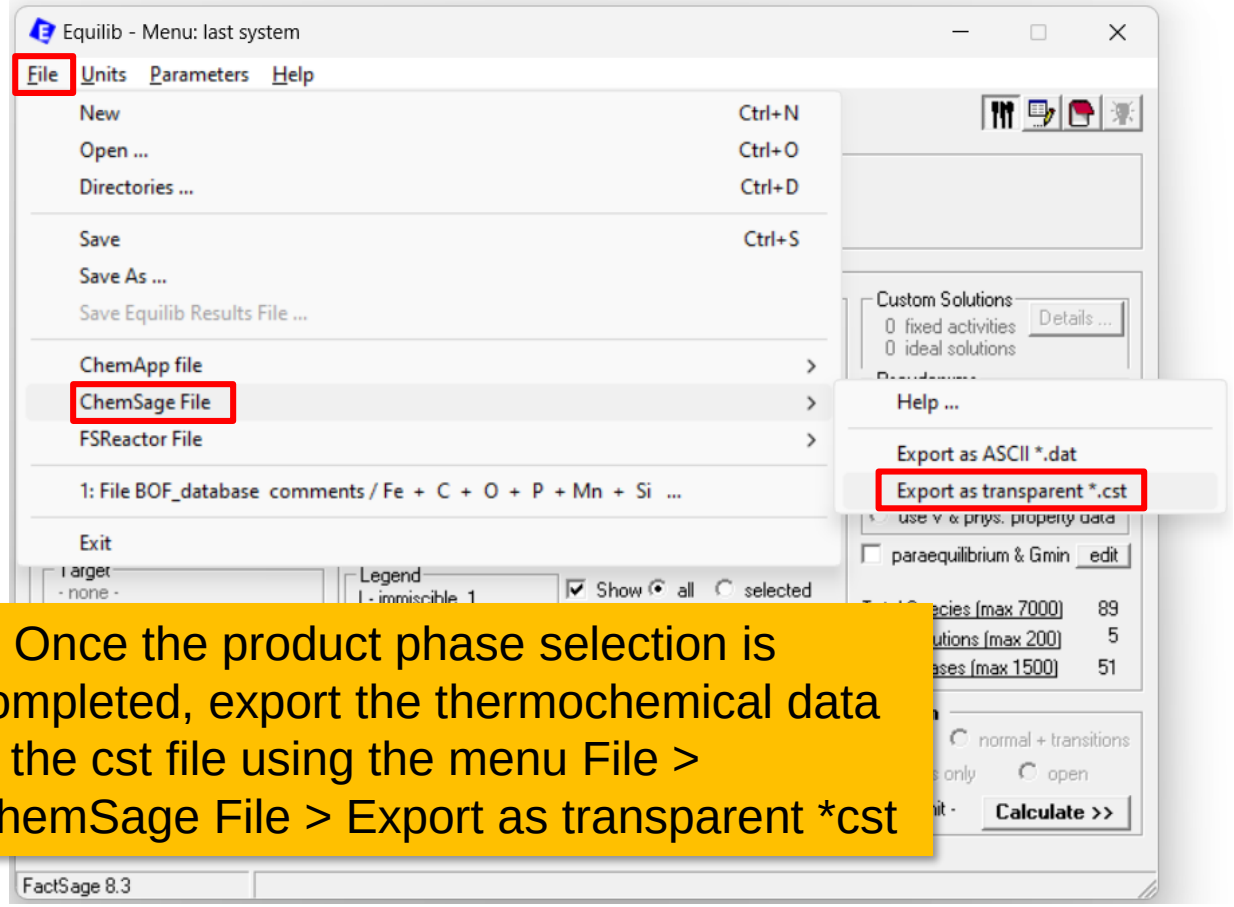
➢ From reactants and phase selection



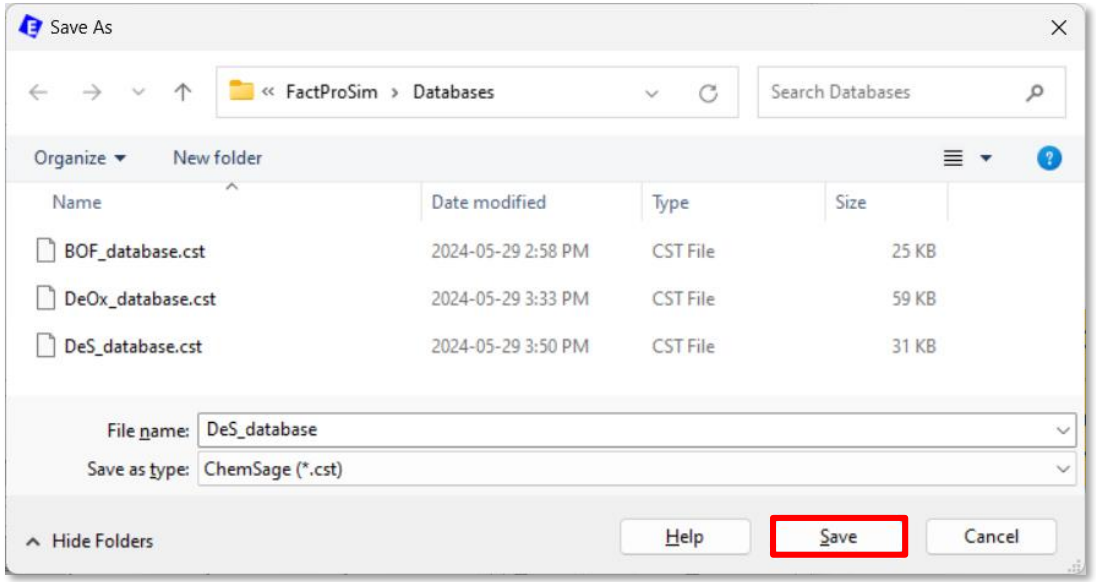
3. Select the product compound species (gas, pure liquids and pure solids) and solution phases
   - Final conditions and calculations are not required
   - Make sure to select all the desired phases to be stored in the cst file

Step 1: Create a database file

➢ From reactants and phase selection



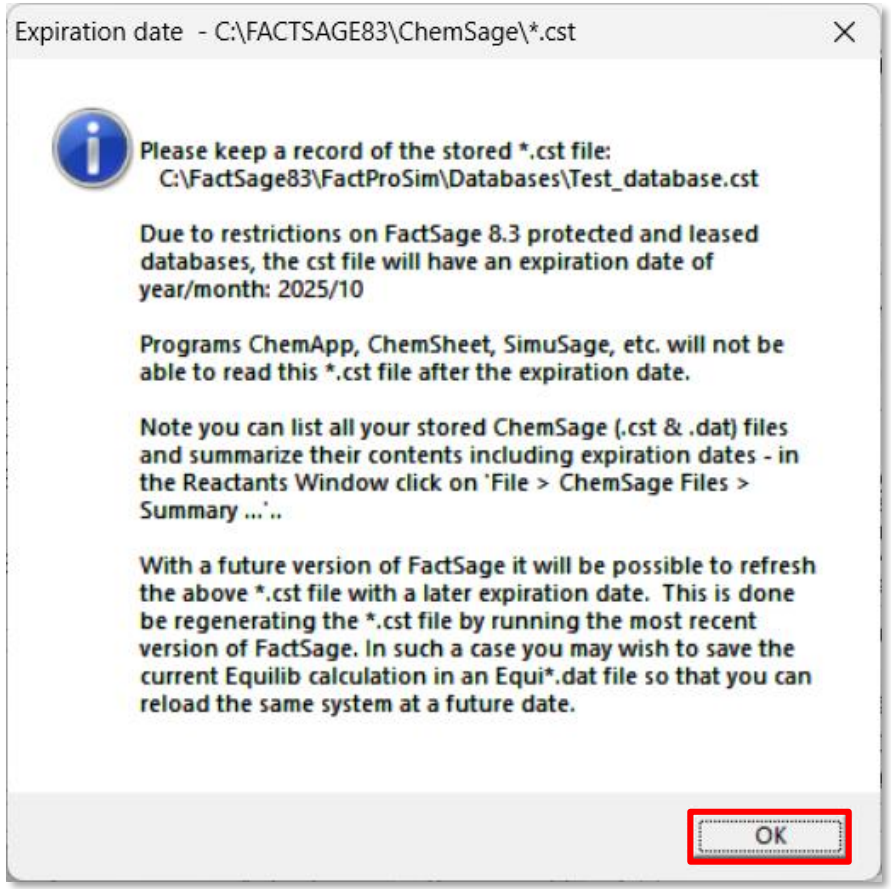
4. Once the product phase selection is completed, export the thermochemical data in the cst file using the menu File > ChemSage File > Export as transparent *cst



5. Choose the location and name for the cst file

Step 1: Create a database file

➢ From reactants and phase selection



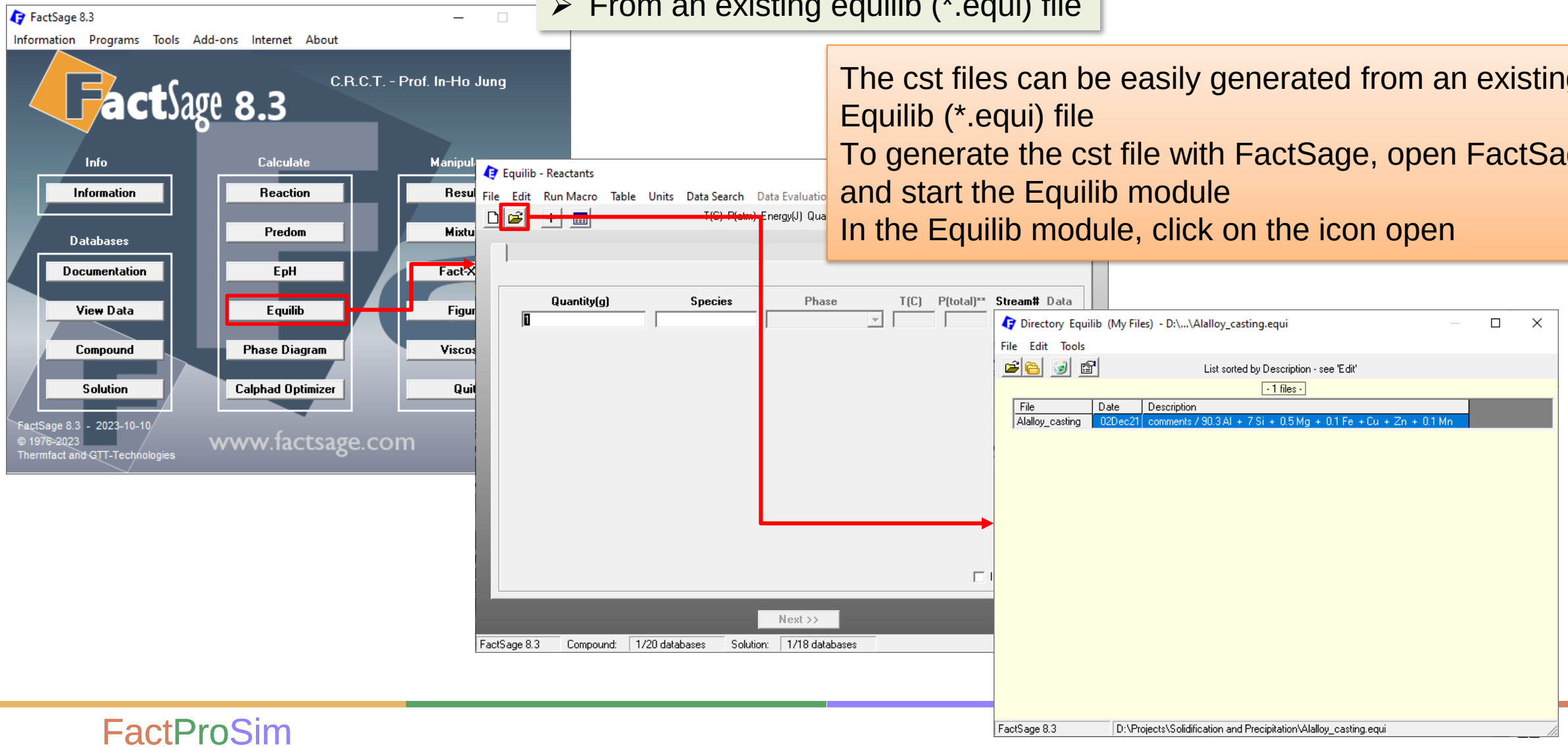
6. The cst files have an expiration date set by FactSage, after which the file will not be readable by FactProSim (and other ChemApp-based programs)

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

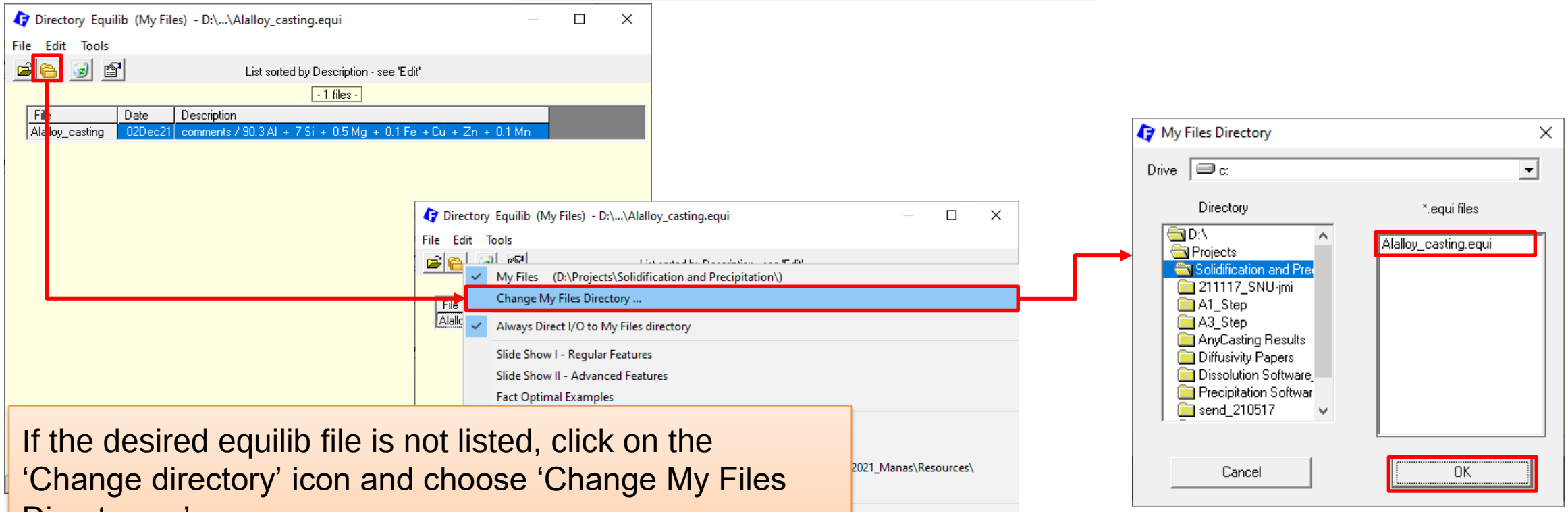
- From an existing equilib (*.equi) file

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



Step 1: Create a database file

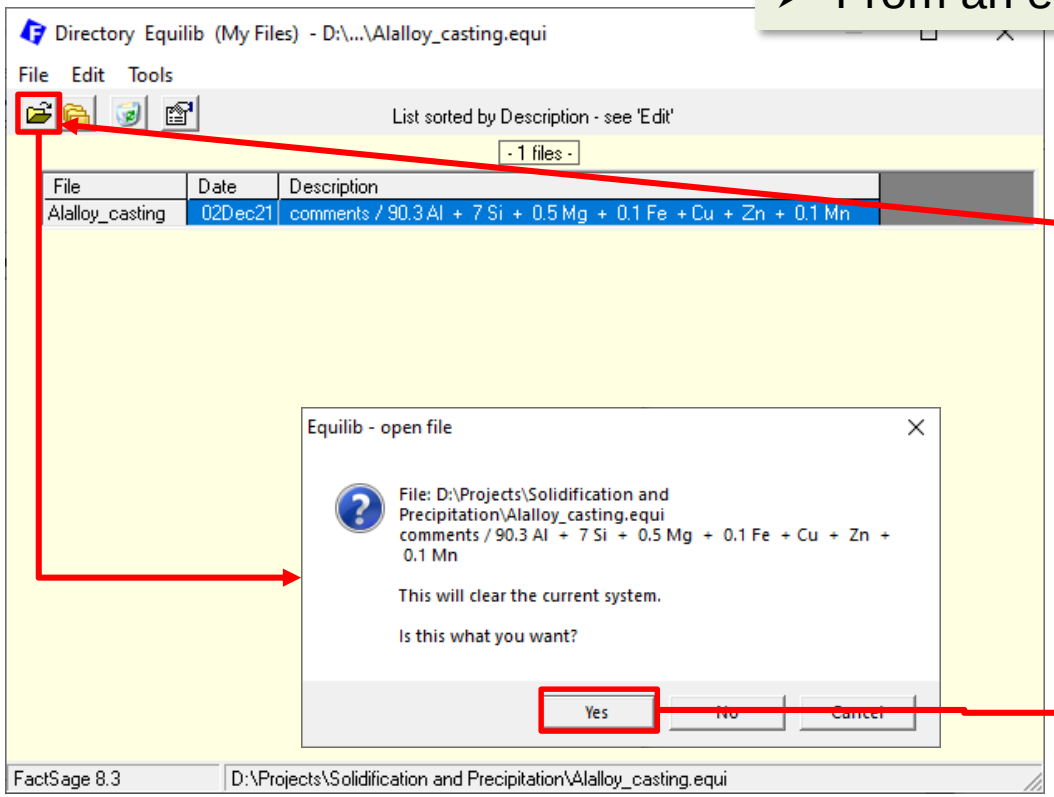
➢ From an existing equilib (*.equi) file



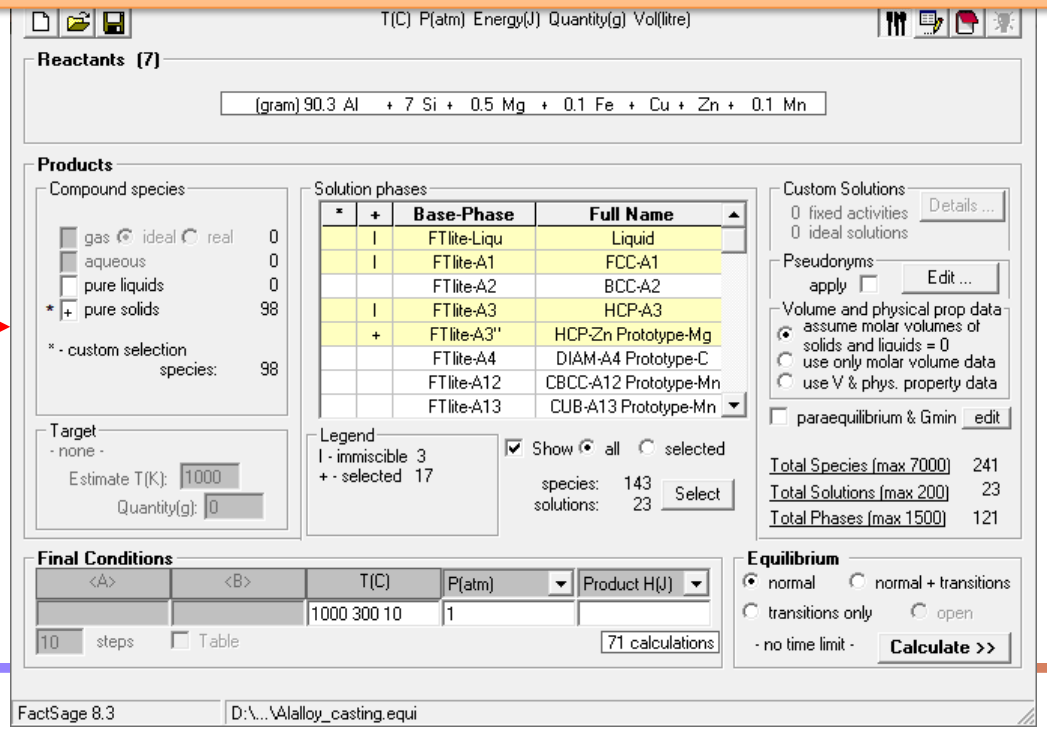
If the desired equilib file is not listed, click on the 'Change directory' icon and choose 'Change My Files Directory…'
The 'My Files Directory' dialog window opens.
Browse the directories and select the desired folder where the *.equi file is located. Click 'OK'

Step 1: Create a database file

➢ From an existing equilib (*.equi) file

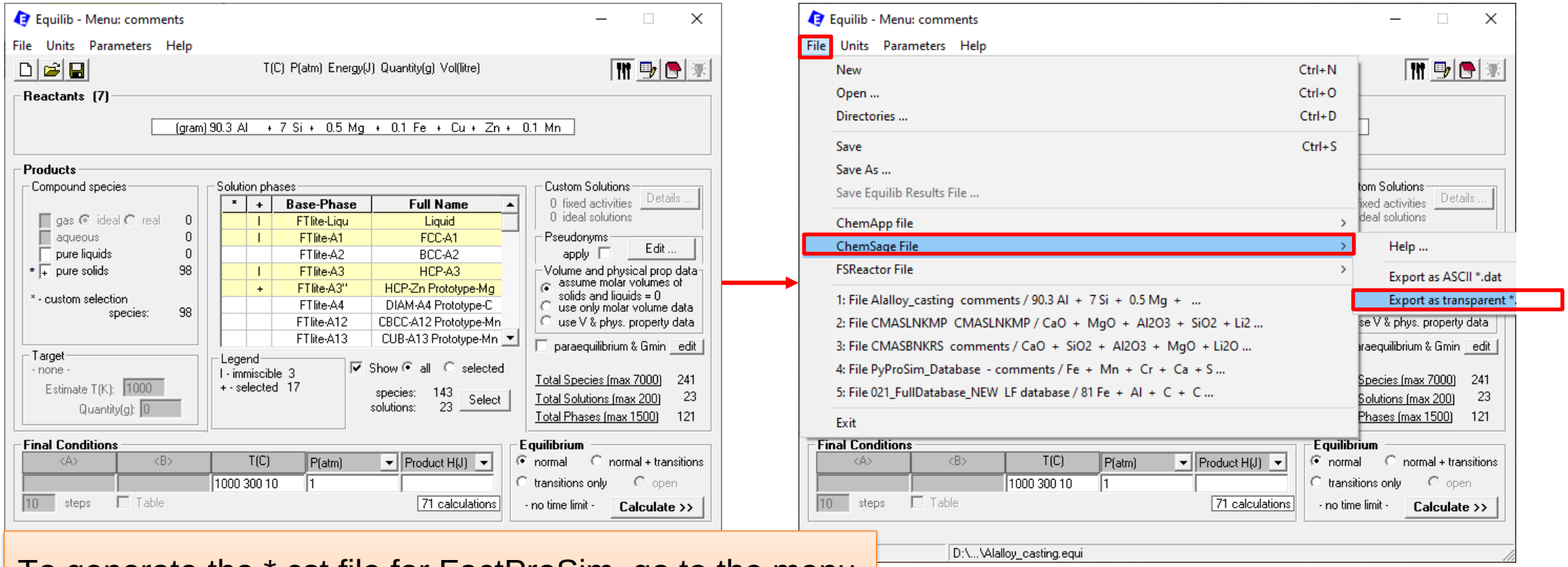


Select the desired .equi file in the list
Double-click or select the icon ‘Open’ to load the equilib file in the Equilib module
Click ‘Yes’ in the dialog box to clear the current system and load the one saved in the file



Step 1: Create a database file

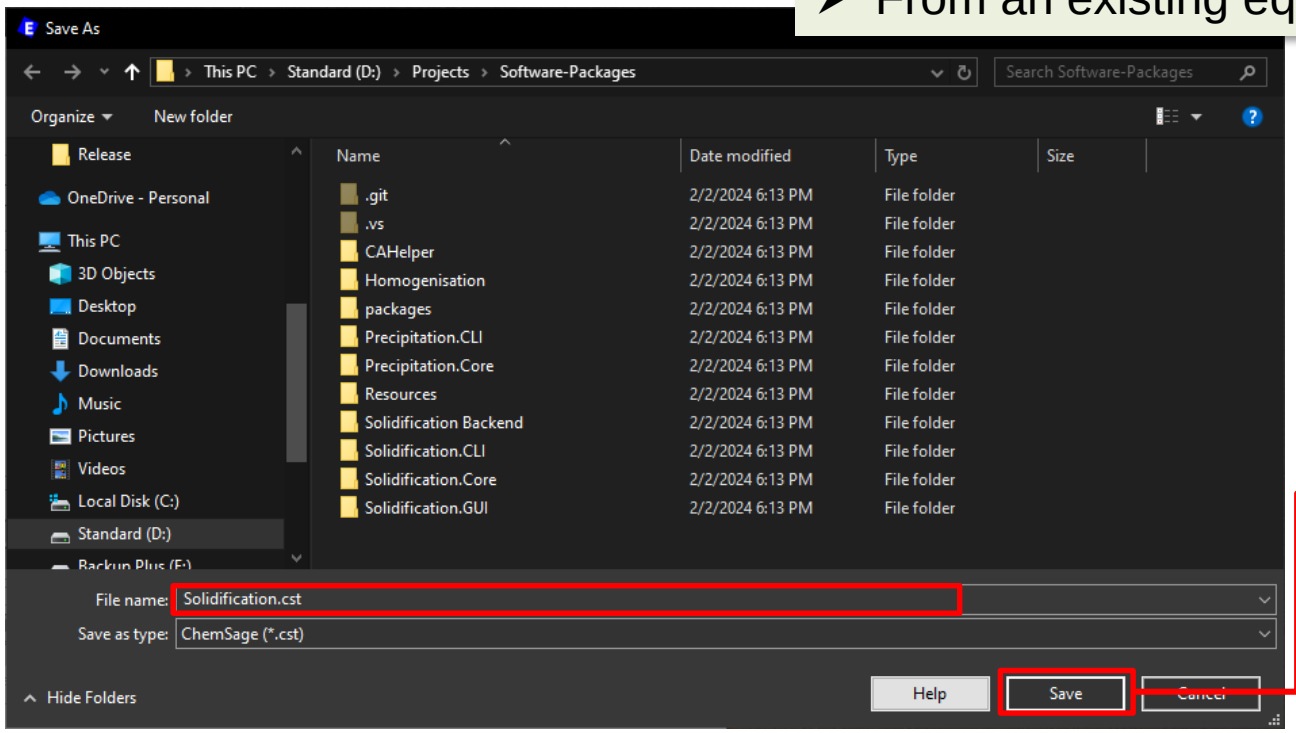
➢ From an existing equilib (*.equi) file

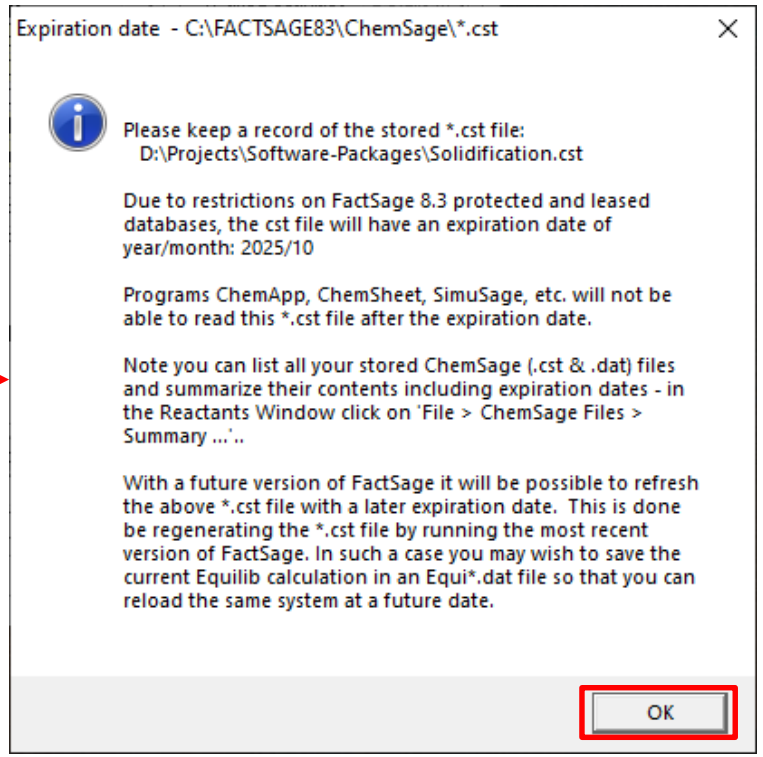


To generate the *.cst file for FactProSim, go to the menu window of Equilib. In the ‘File’ menu, select ‘ChemSage File’, then ‘Export as transparent *.cst’

Step 1: Create a database file

➢ From an existing equilib (*.equi) file



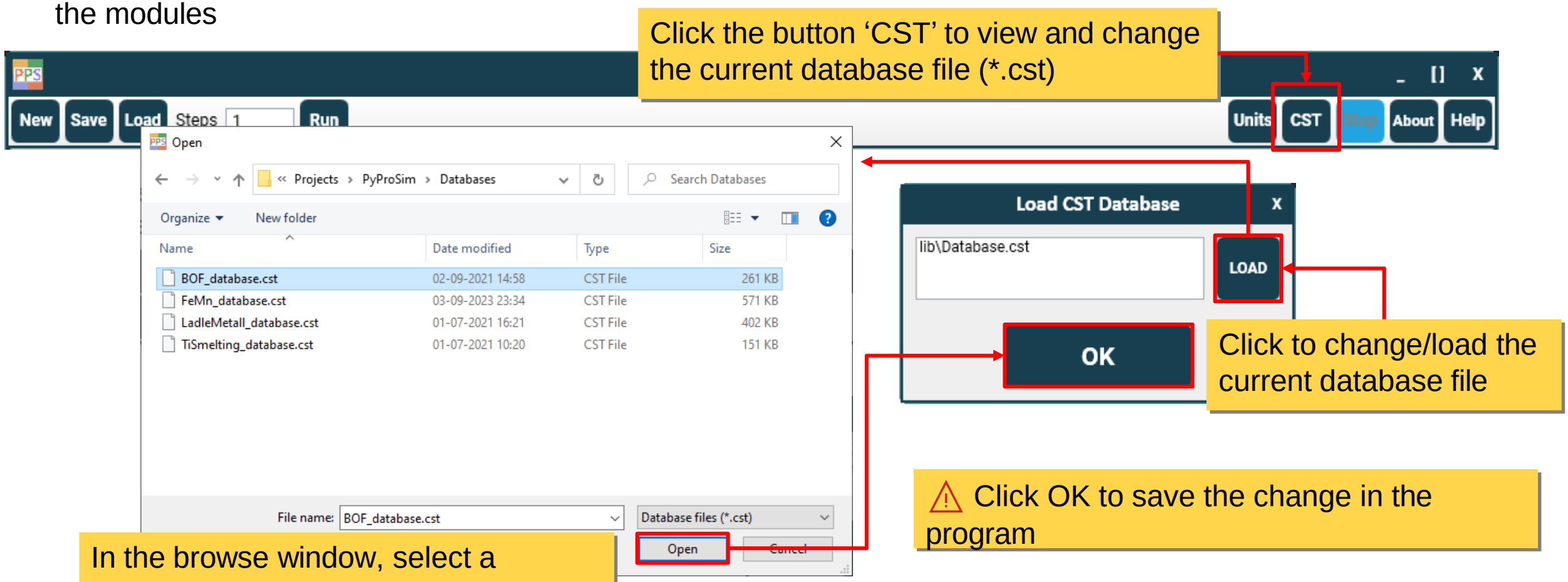


It will open a save dialog window, where the location and name of the cst file can be entered. Click “Save”

⚠ 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



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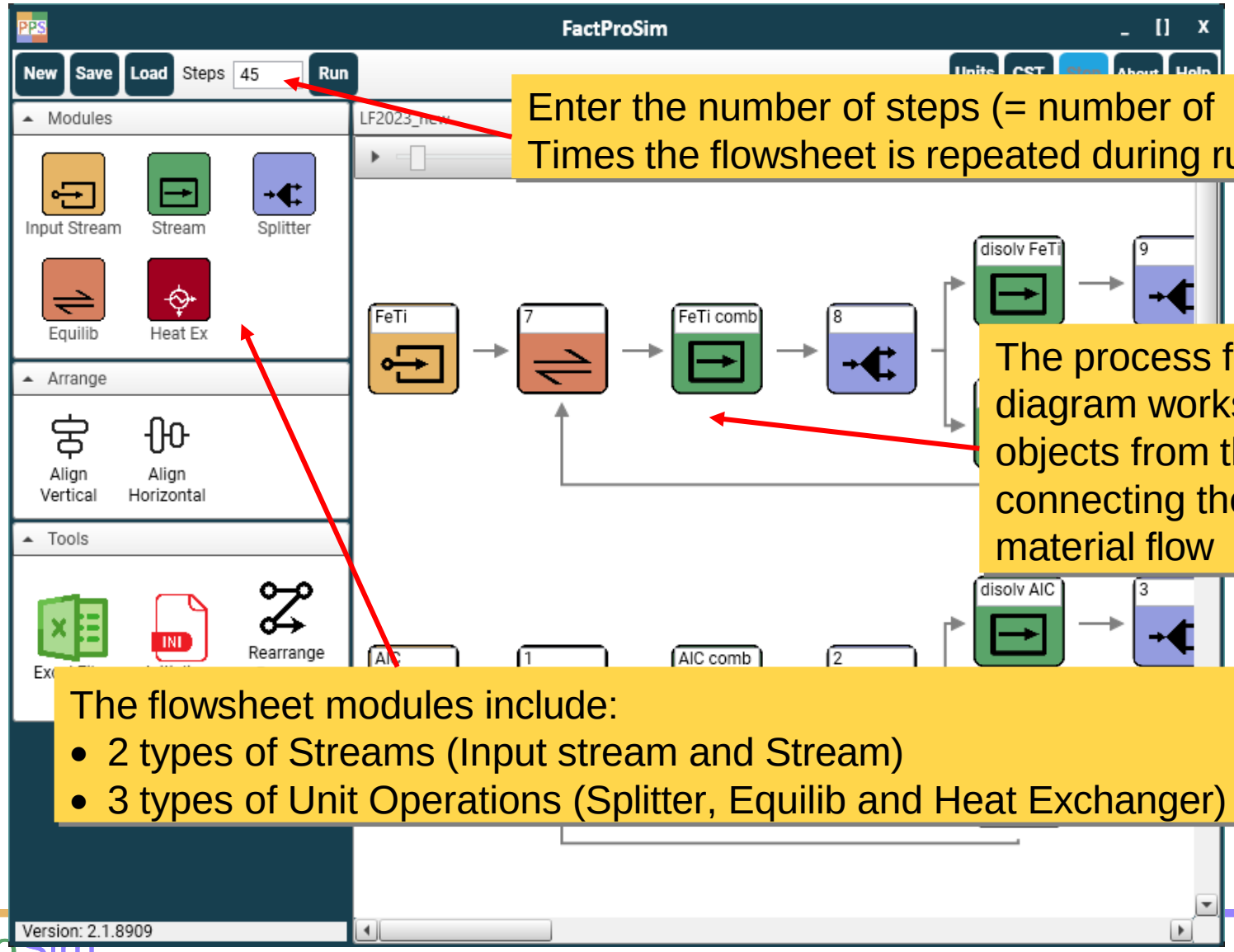
Step 2: Build the process flowsheet



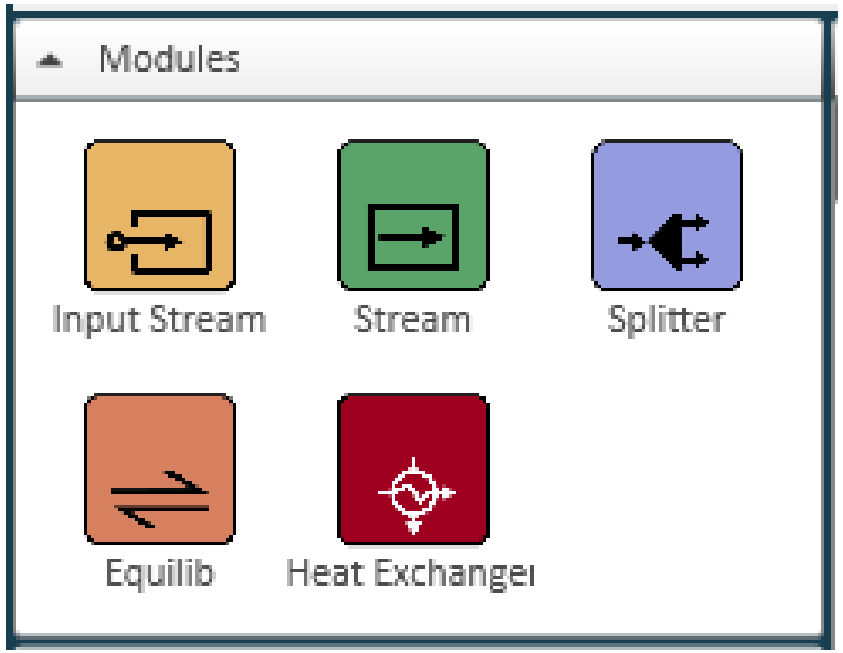
Enter the number of steps (= number of Times the flowsheet is repeated during run)

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)

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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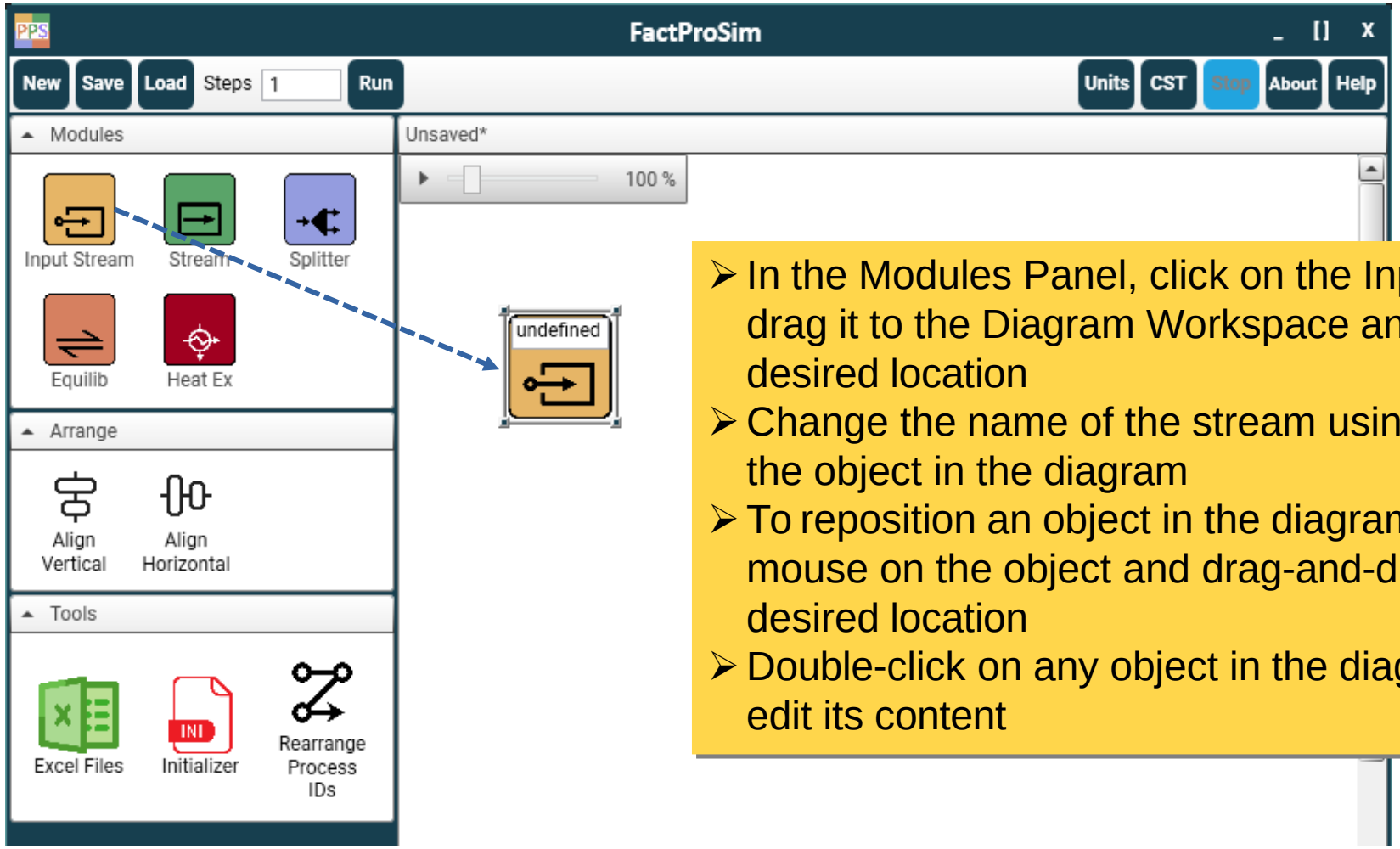
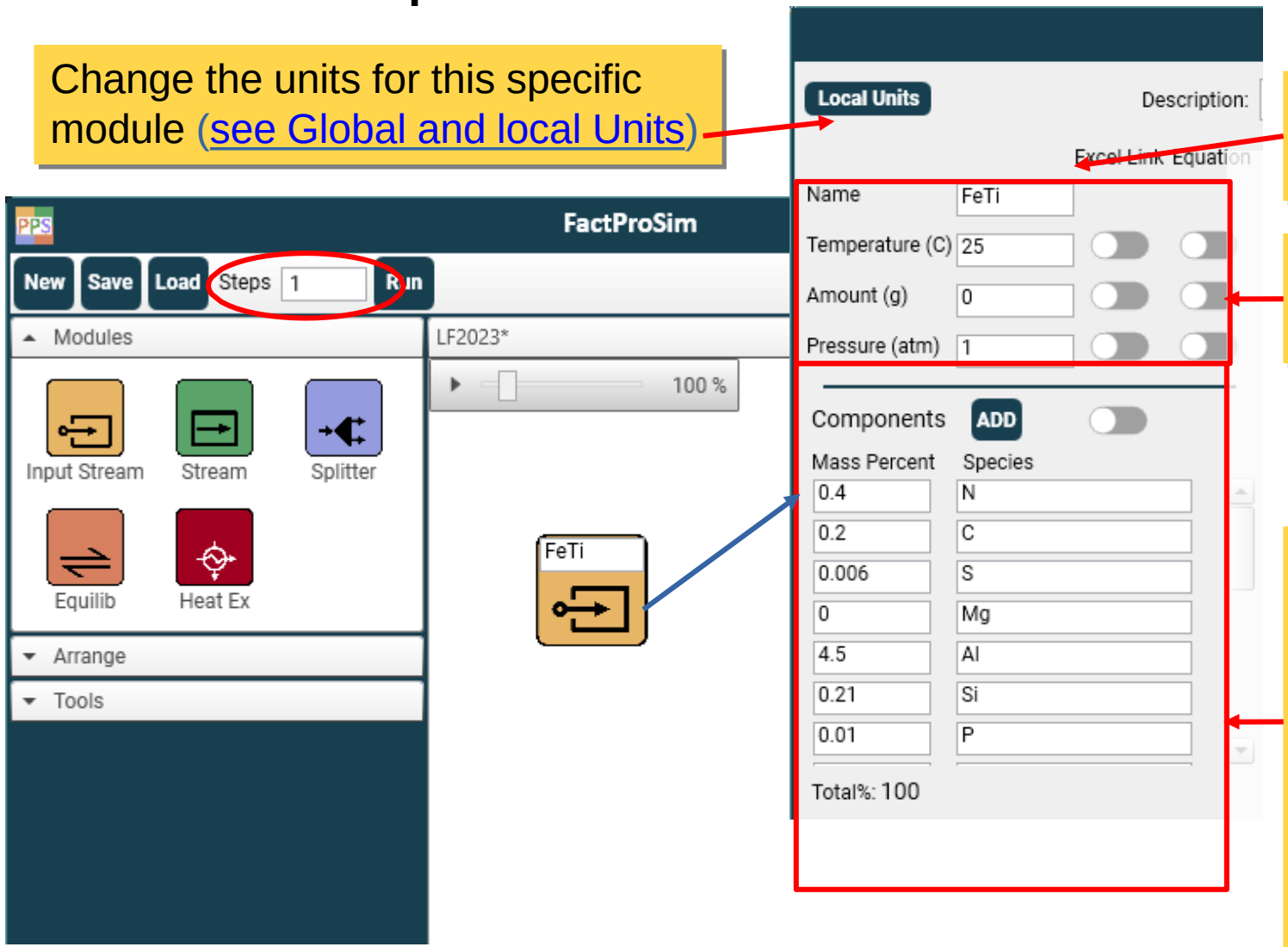
Adding an Input Stream in the diagram



- 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)

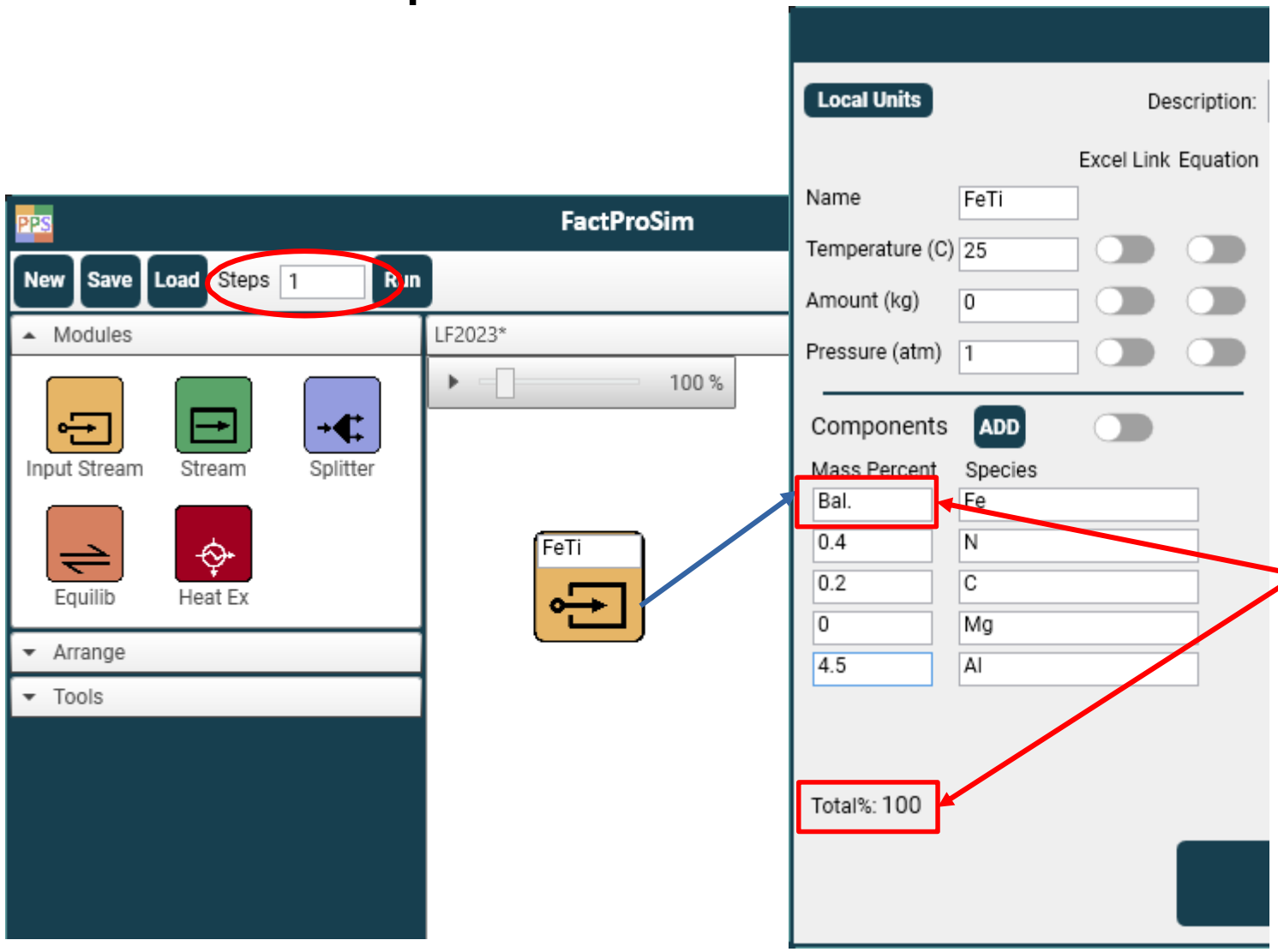


Change the name of the stream (same function from the module textbox)

Enter the Temperature, Amount and Pressure

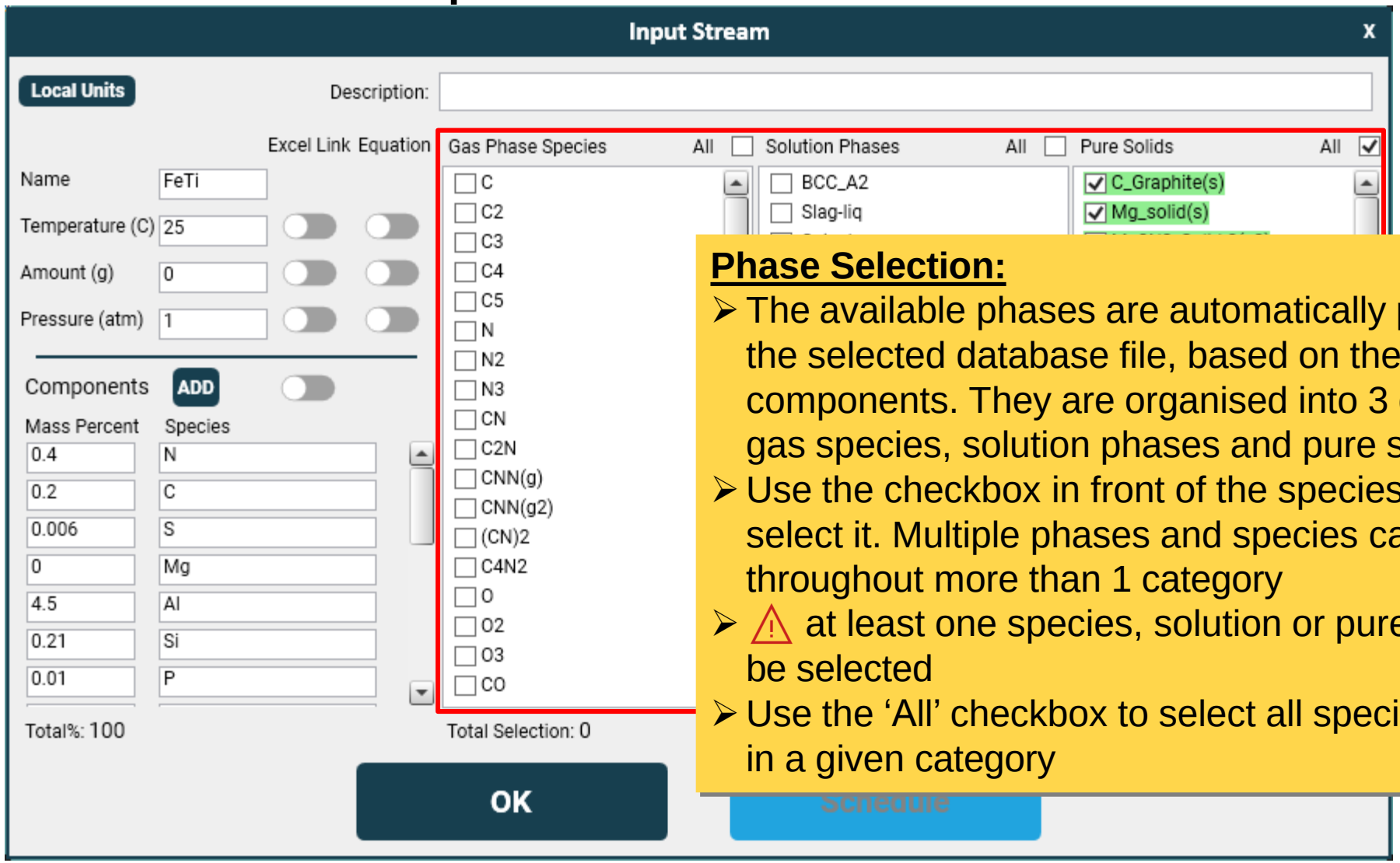
- List all the components (chemical formula only, ex: Fe, CaO) and their composition (in percentage), 1 component per line
- Press the button 'Add' to add a new component (new line)
- The total content is indicated at the bottom

Input Stream Module – Manual entry, 1 step



The “Bal.” keyword will automatically assign the remaining mass/mole to the corresponding element, and make the sum of the composition equal to “100”

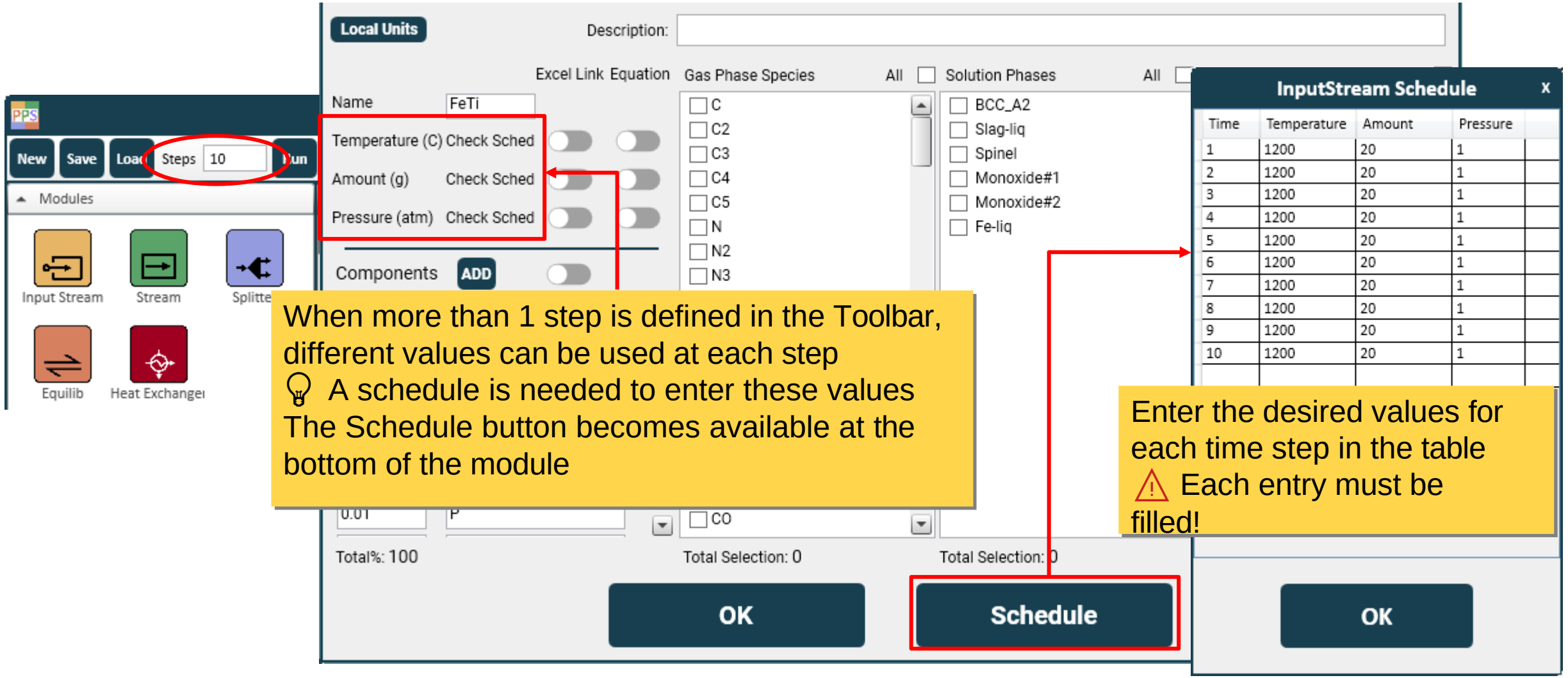
Input Stream Module – Phase selection



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



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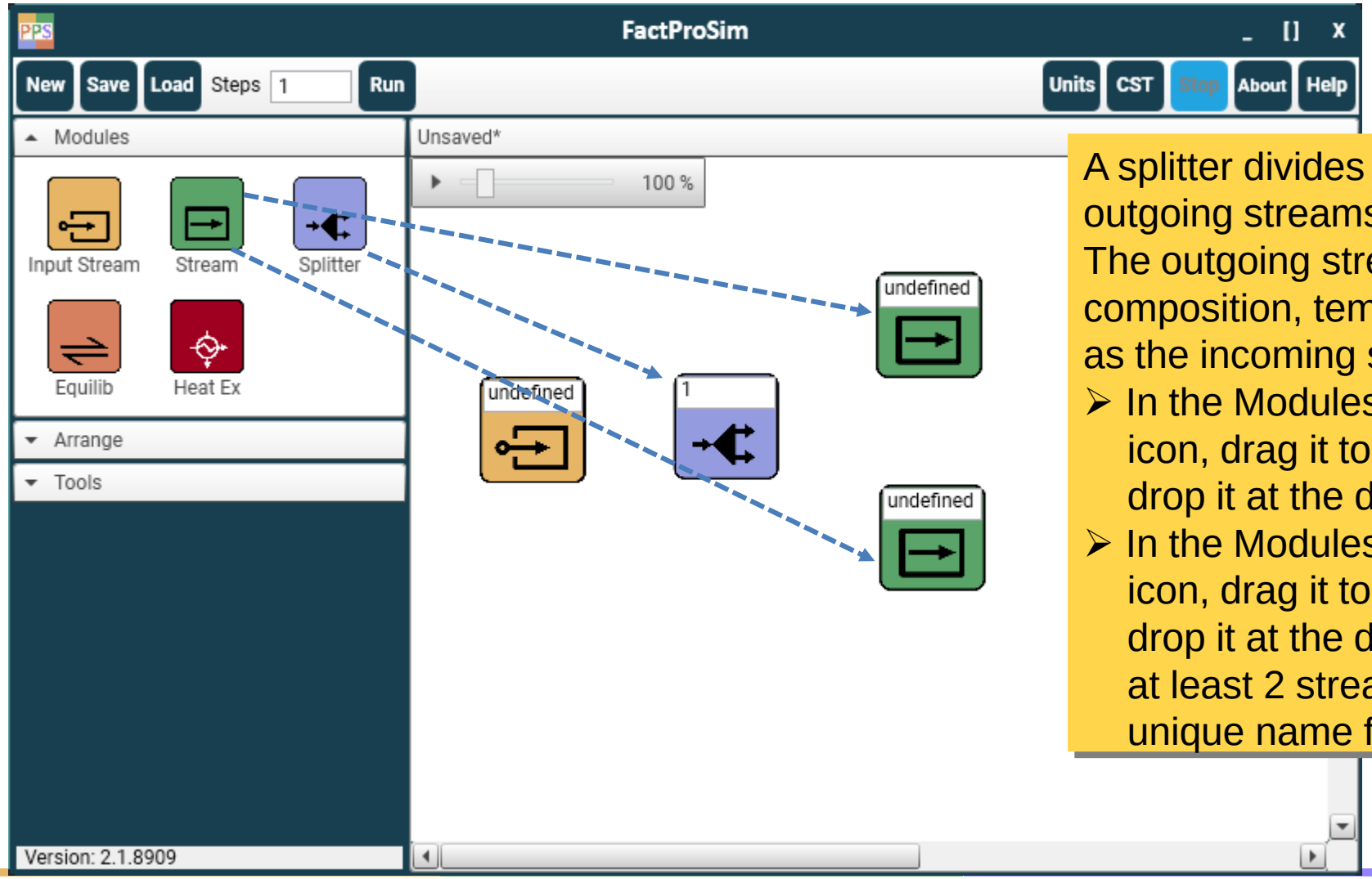
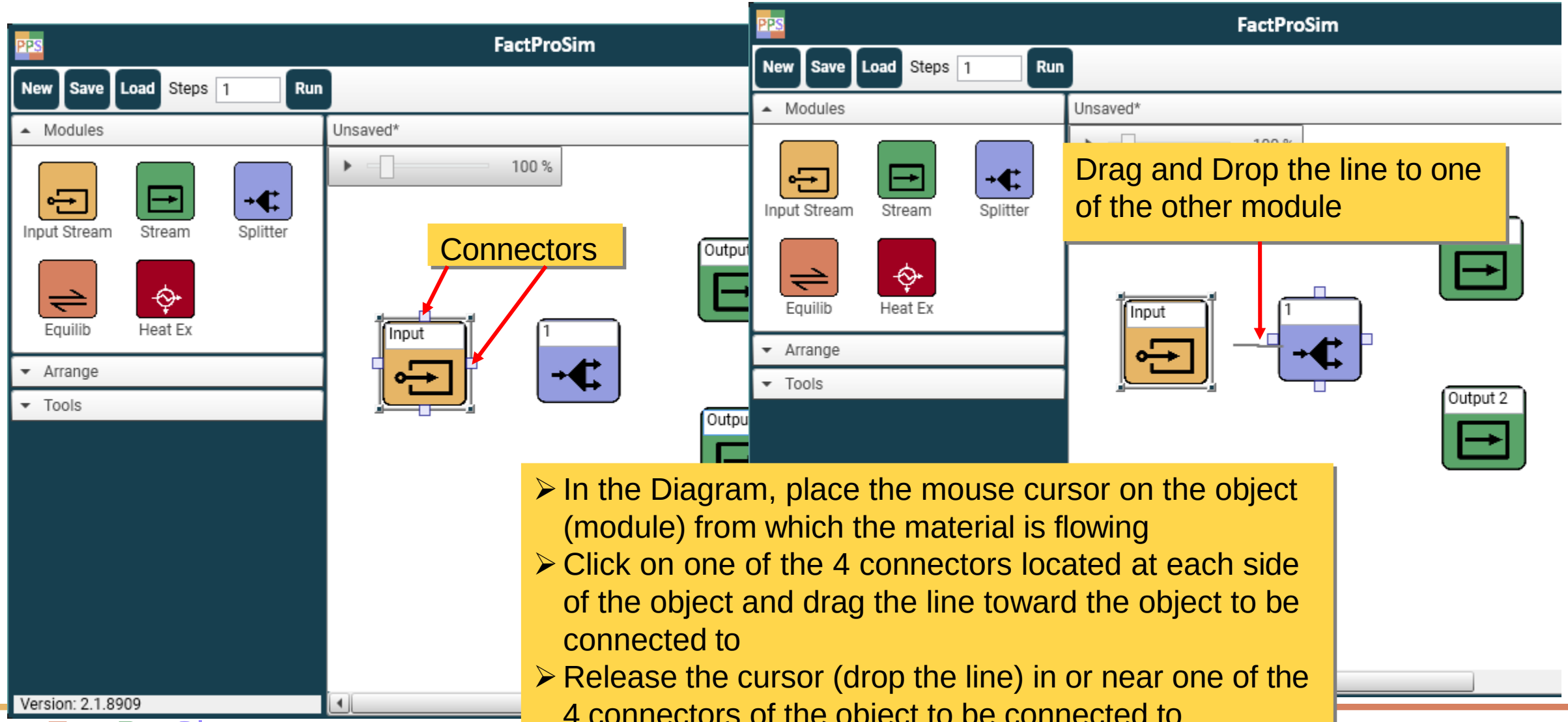
Adding a Splitter and streams in the diagram



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

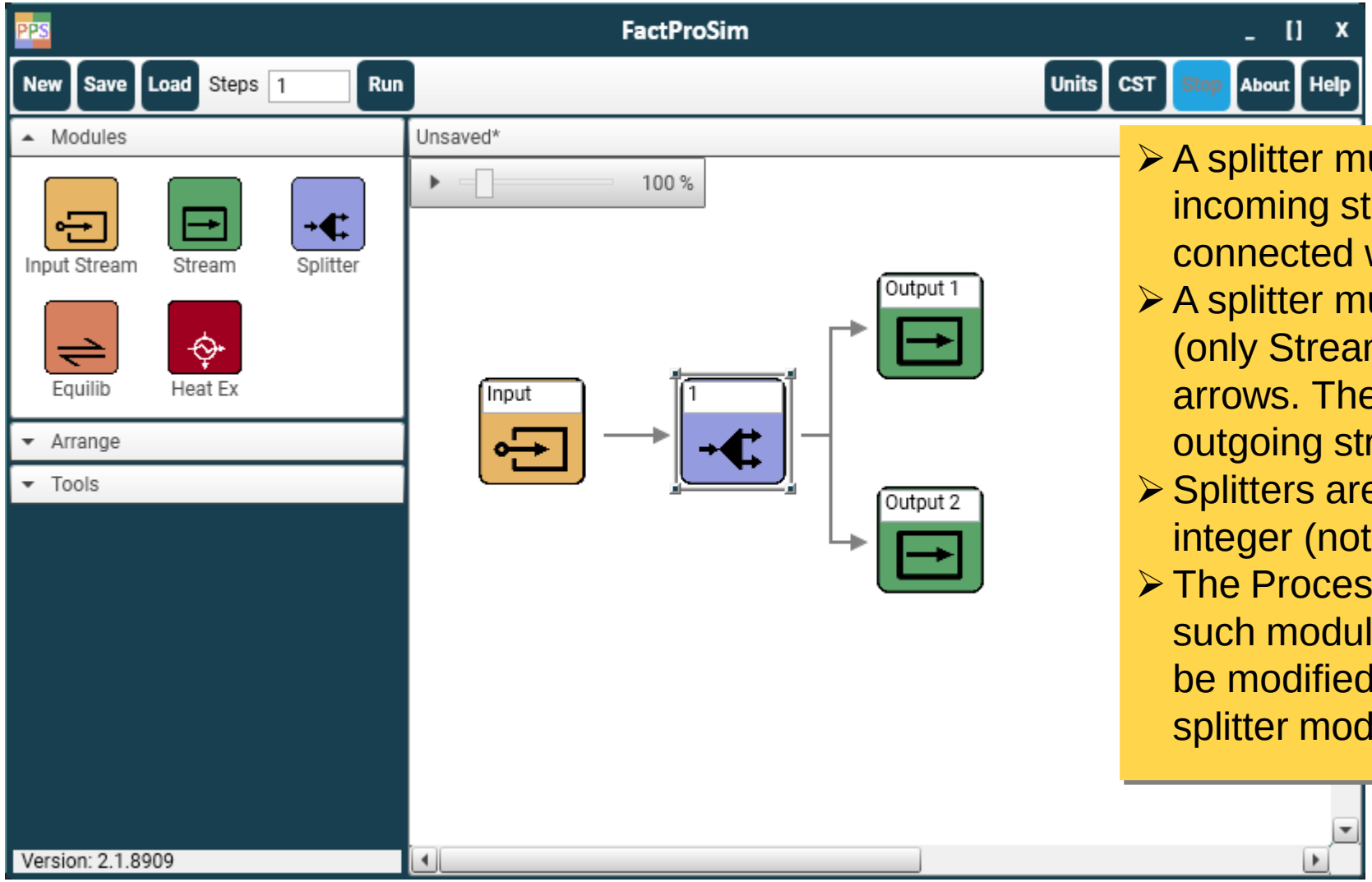
- In the Modules Panel, click on the Splitter icon, drag it to the Diagram Workspace and drop it at the desired location
- In the Modules Panel, click on the Stream icon, drag it to the Diagram Workspace and drop it at the desired location. Repeat to have at least 2 streams in the diagram. Enter a unique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

Connecting modules with arrows (Material flow)



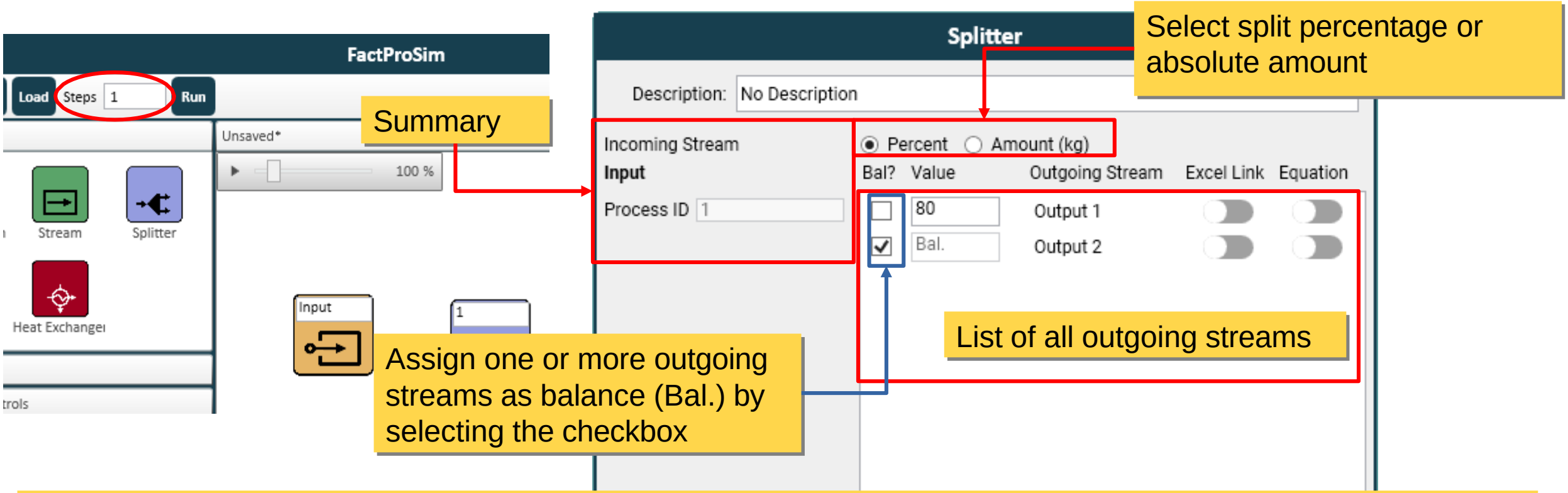
- In the Diagram, place the mouse cursor on the object (module) from which the material is flowing
- Click on one of the 4 connectors located at each side of the object and drag the line toward the object to be connected to
- Release the cursor (drop the line) in or near one of the 4 connectors of the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

Adding a Splitter and streams in the diagram



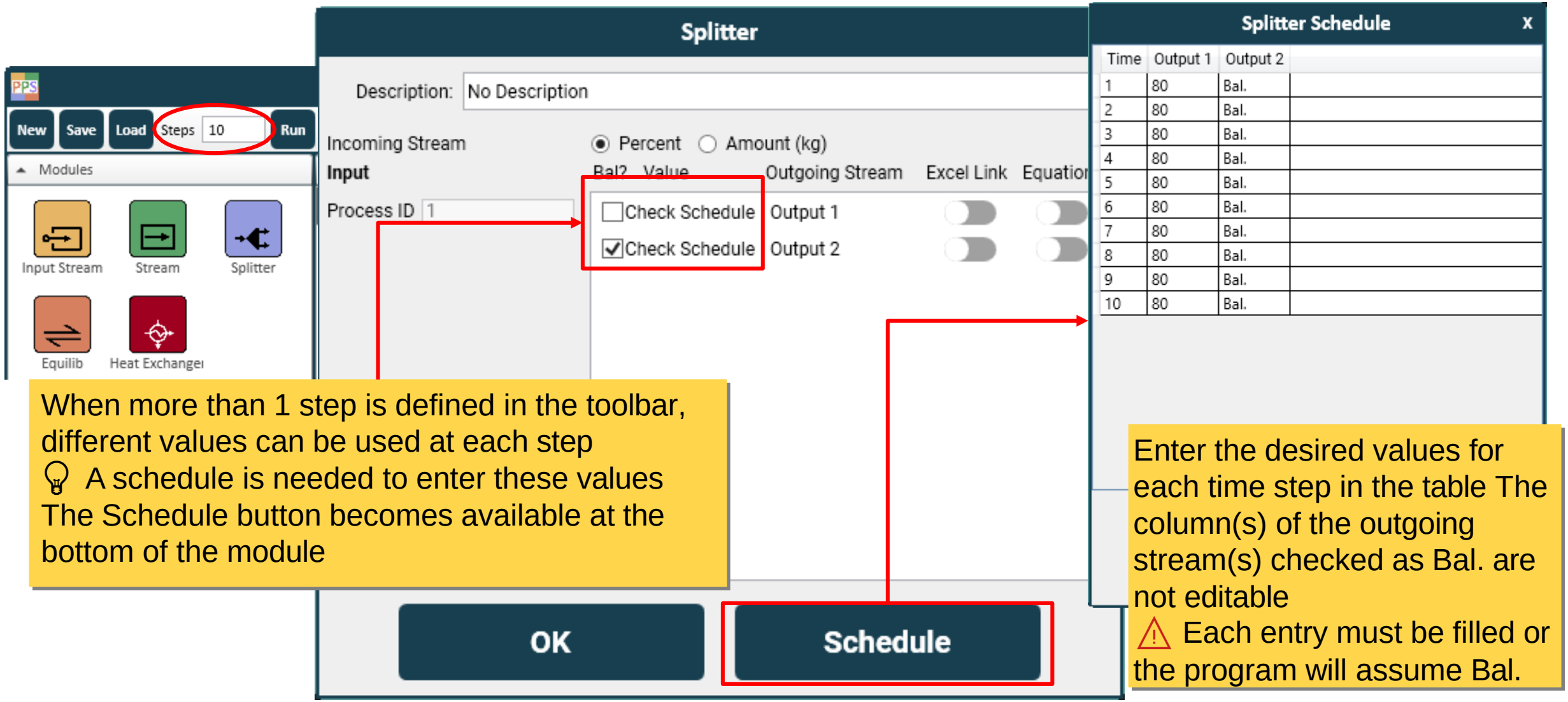
- A splitter must have one **(and only one)** incoming stream (Input Stream or Stream) connected with an inbound arrow
- A splitter must have at least 1 outgoing stream (only Stream objects) connected with outbound arrows. There is no limit in the number of outgoing streams
- Splitters are identified 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



- 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



When more than 1 step is defined in the toolbar, different values can be used at each step

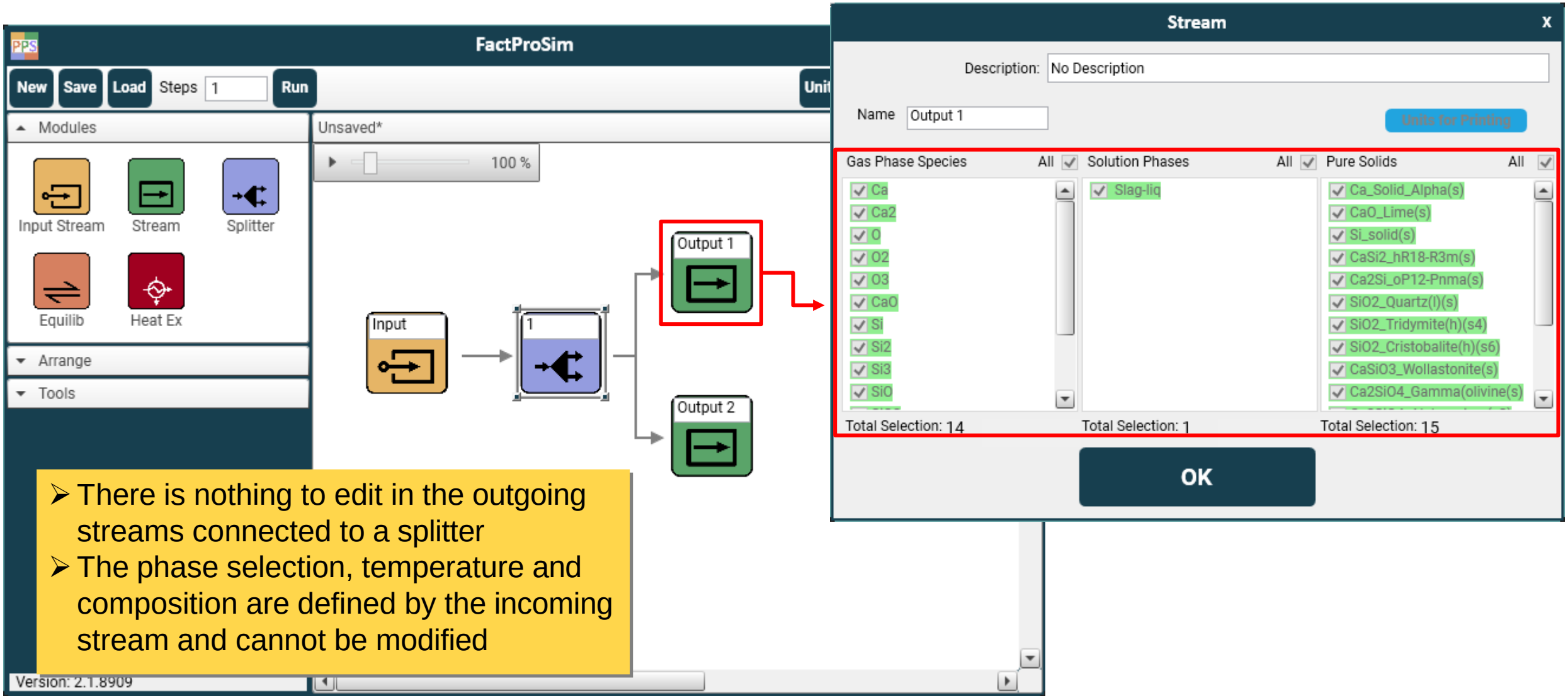
A schedule is needed to enter these values

The Schedule button becomes available at the bottom of the module

Enter the desired values for each time step in the table 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

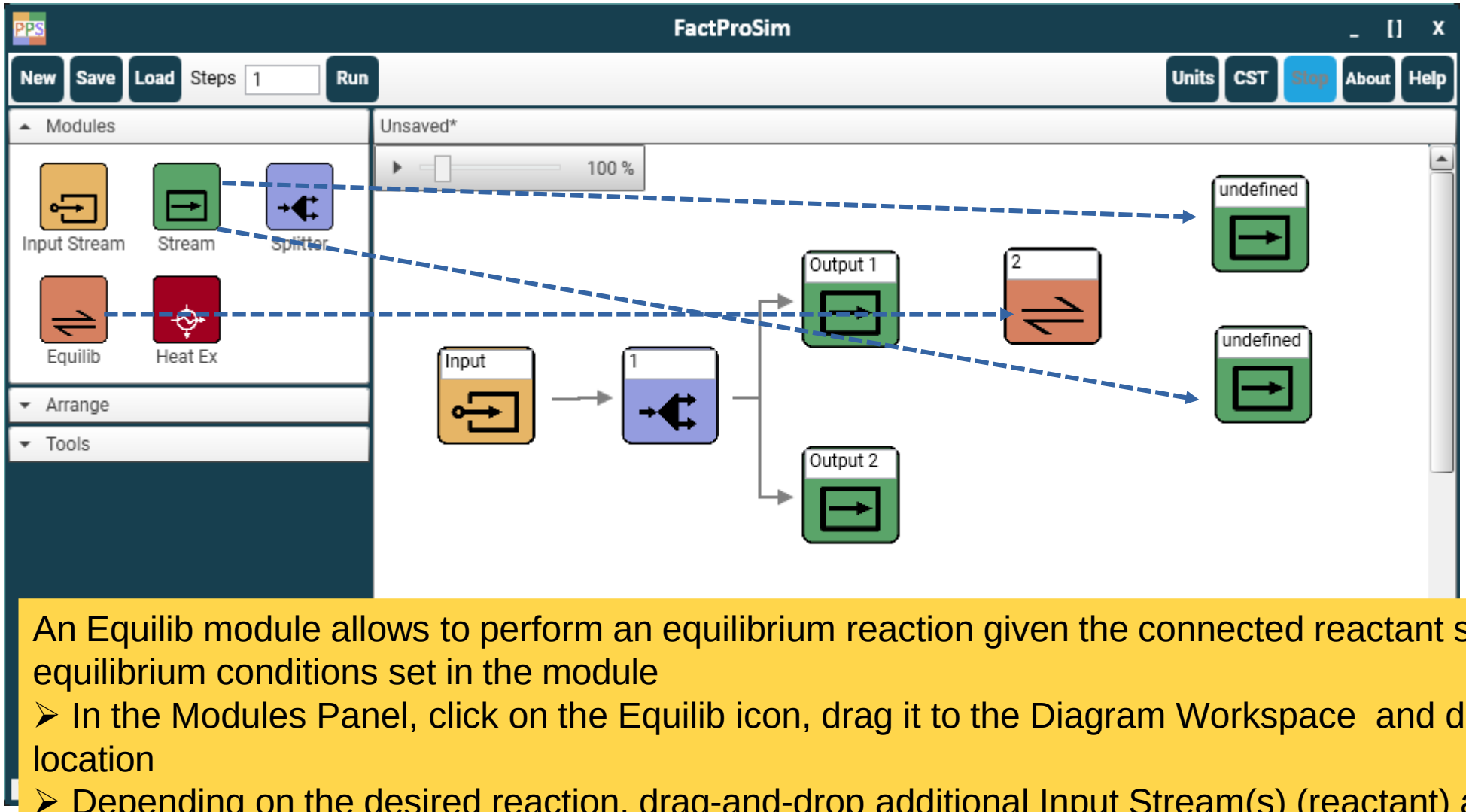


- There is nothing to edit in the outgoing streams connected to a splitter
- The phase selection, temperature and composition are defined by the incoming stream and cannot be modified

Description of the program

- Overview of the main window and commands in the Toolbar
- 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)

Add Equilib module and reactant streams in the diagram

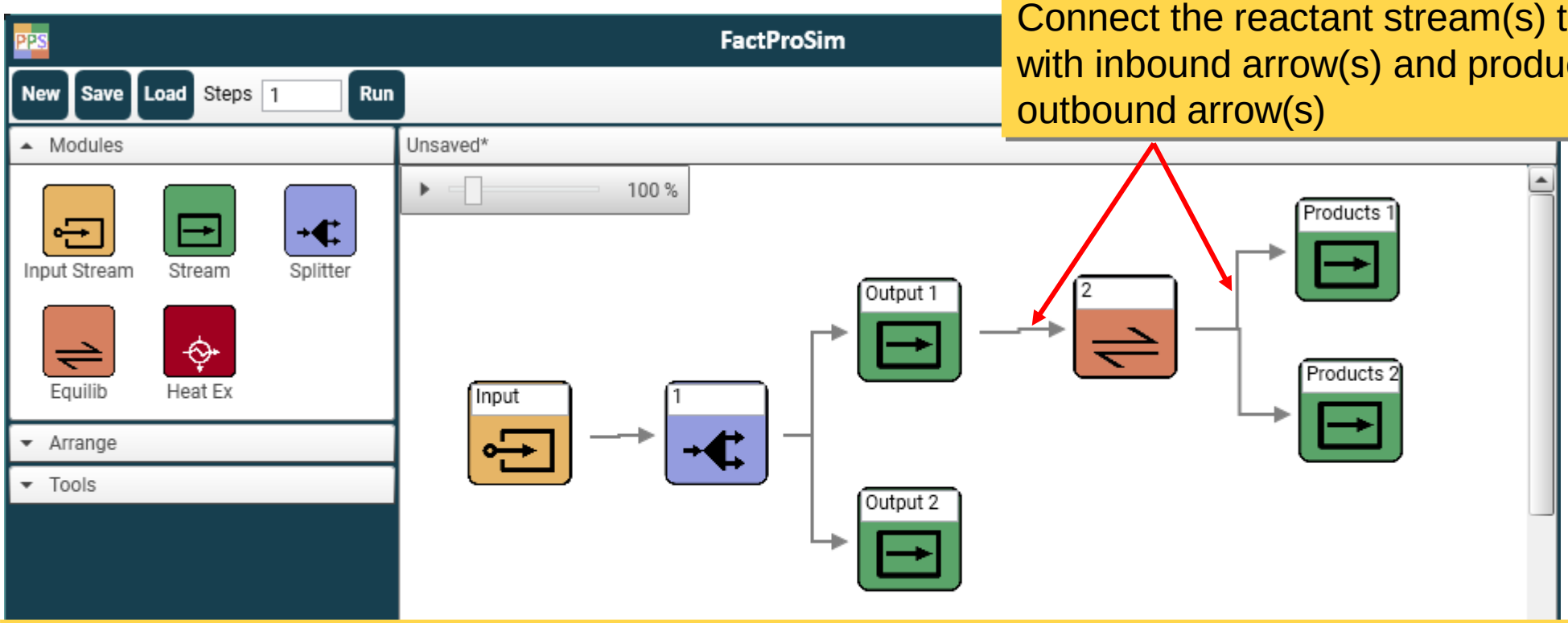


An Equilib module allows to perform an equilibrium reaction given the connected reactant stream(s) and equilibrium conditions set in the module

- 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

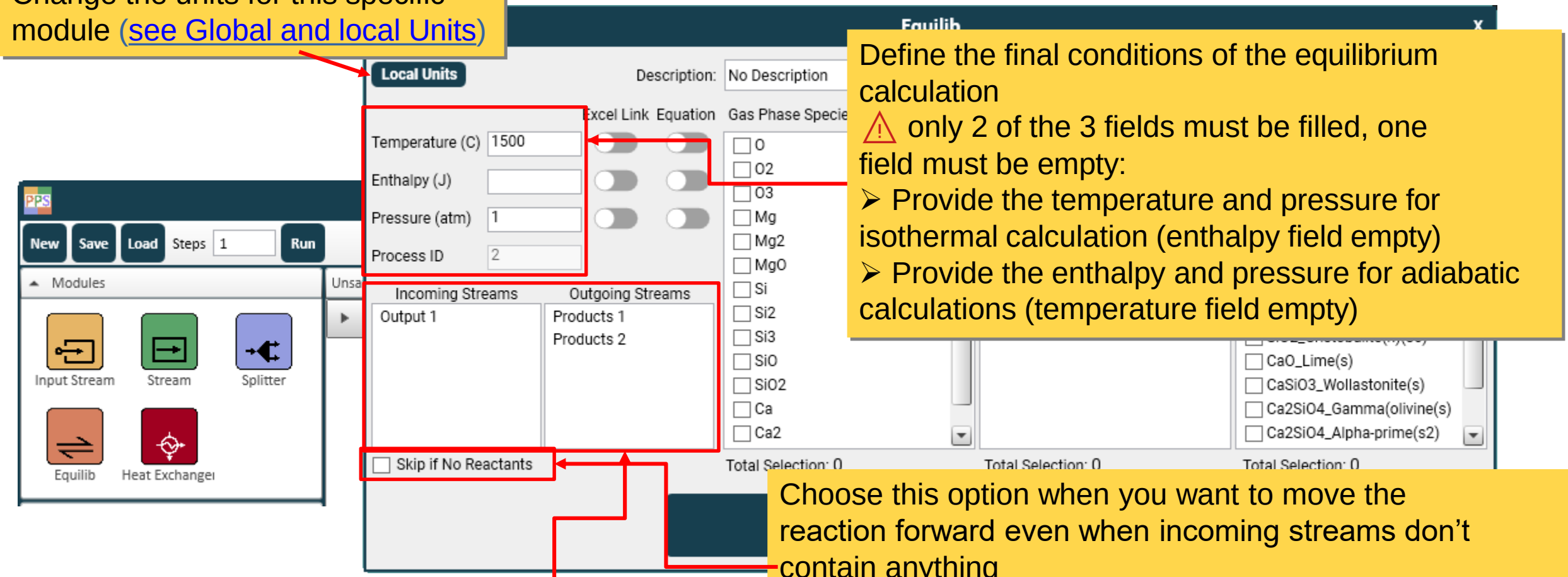
Connect the reactant stream(s) to the Equilib module with inbound arrow(s) and product stream(s) with outbound arrow(s)



- 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)



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)

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

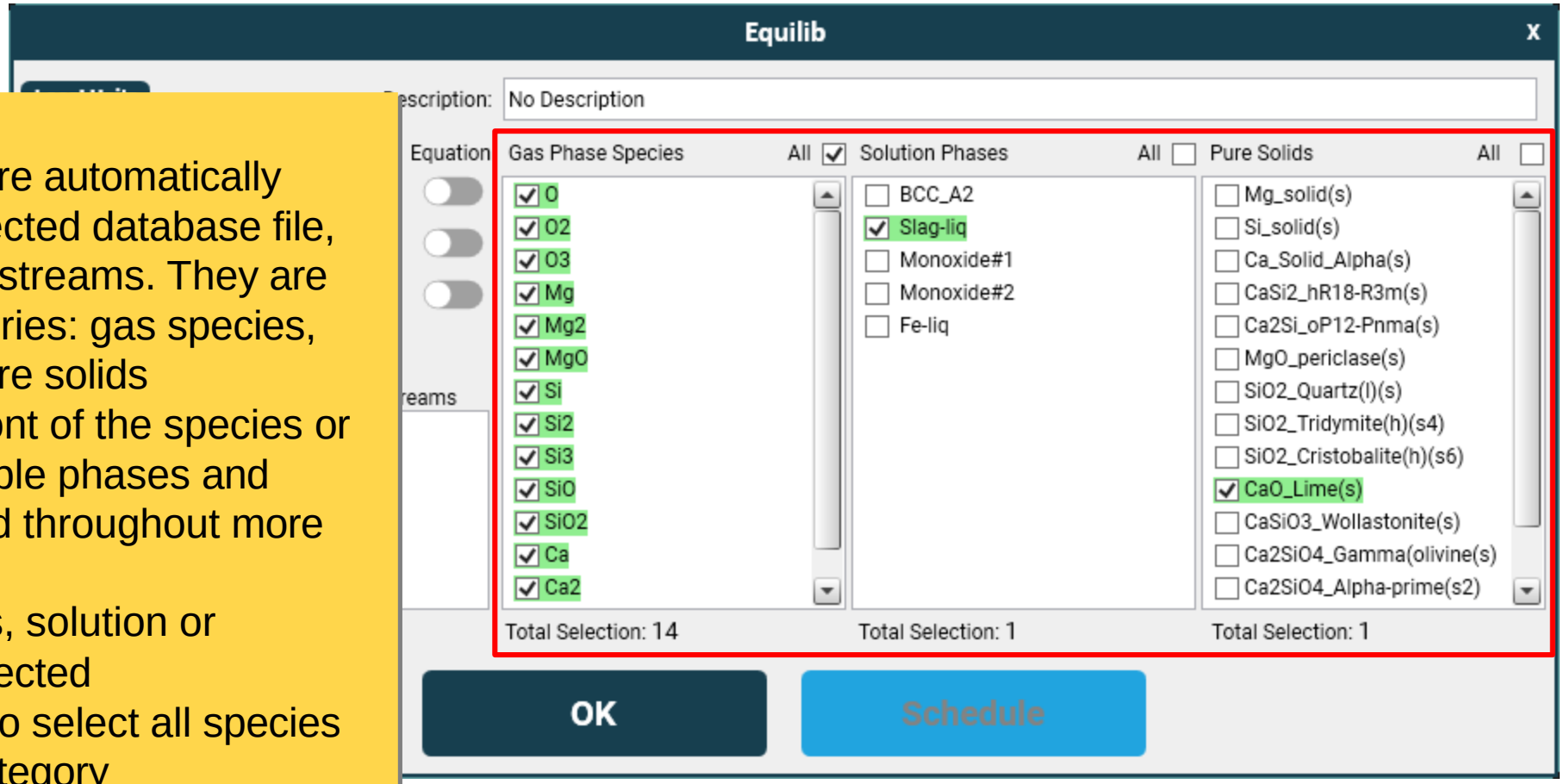
⚠ This is dangerous and should be done fully realizing the effect of it

Summary of incoming and outgoing streams and Process ID

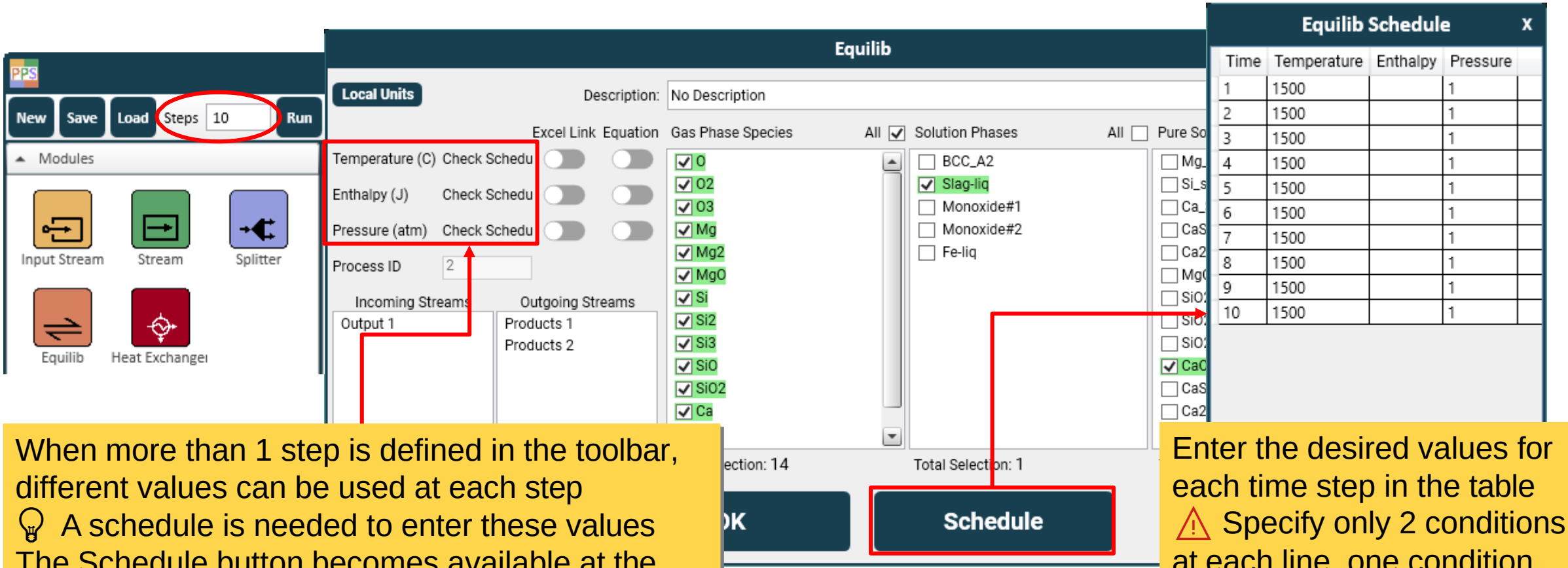
Equilib Module – Manual entry, 1 step

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



Equilib Module – Manual entry, >1 step



When more than 1 step is defined in the toolbar, different values can be used at each step

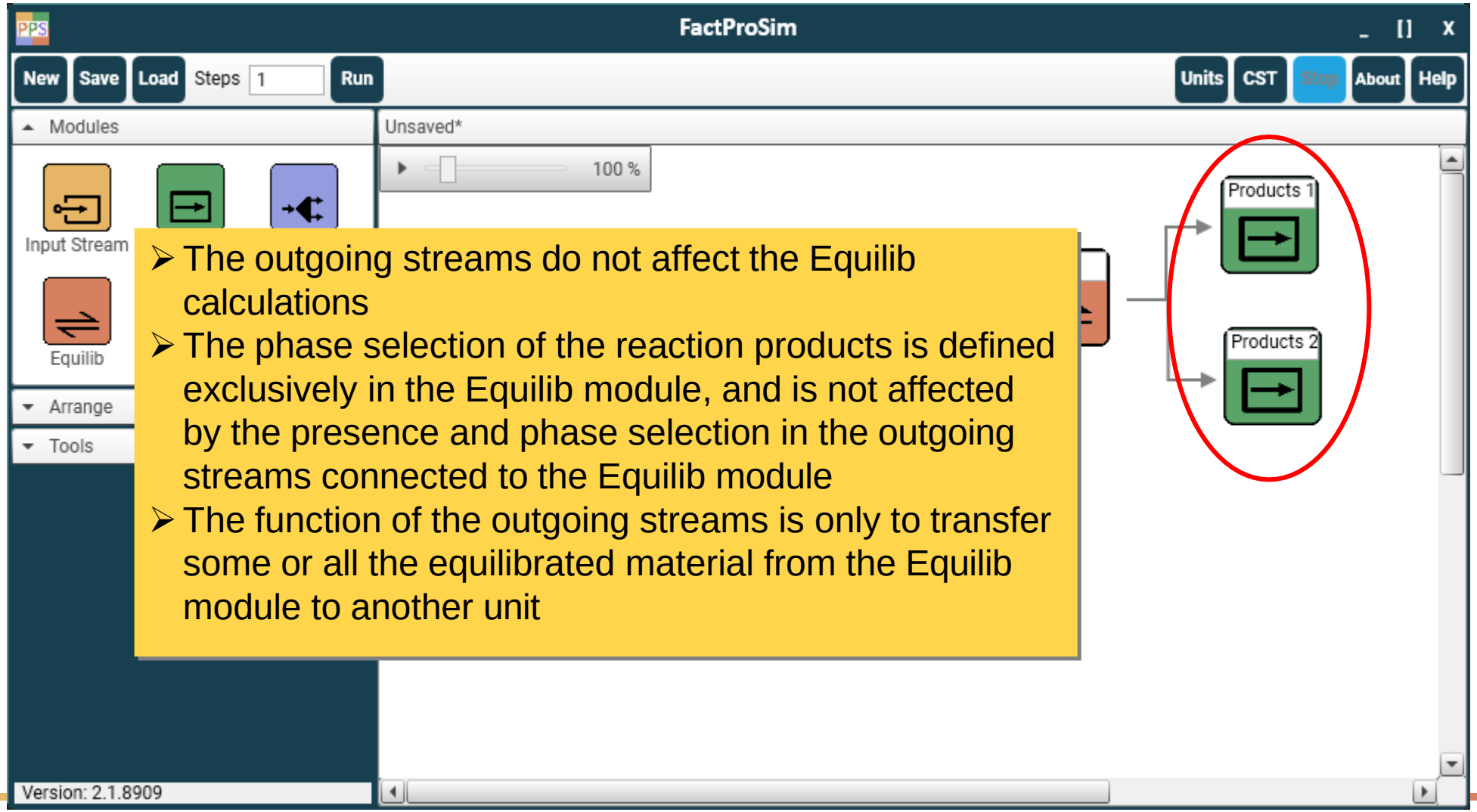
💡 A schedule is needed to enter these values

The Schedule button becomes available at the bottom of the module

Enter the desired values for each time step in the table

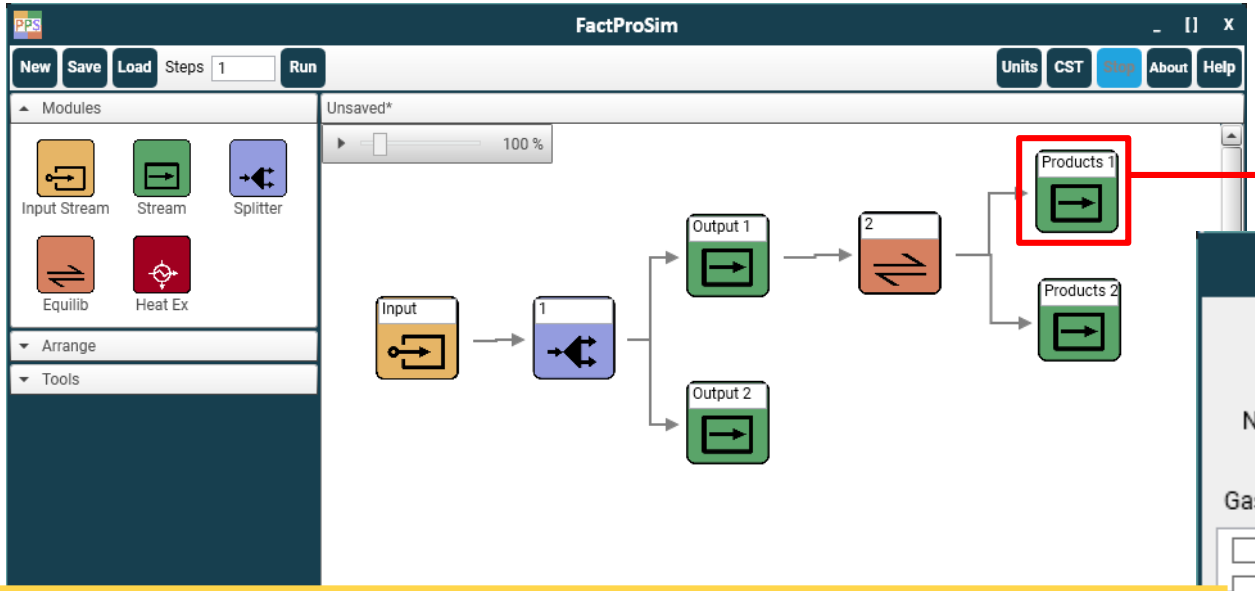
⚠ Specify only 2 conditions at each line, one condition must be empty

Equilib Module – Outgoing streams (reaction products)

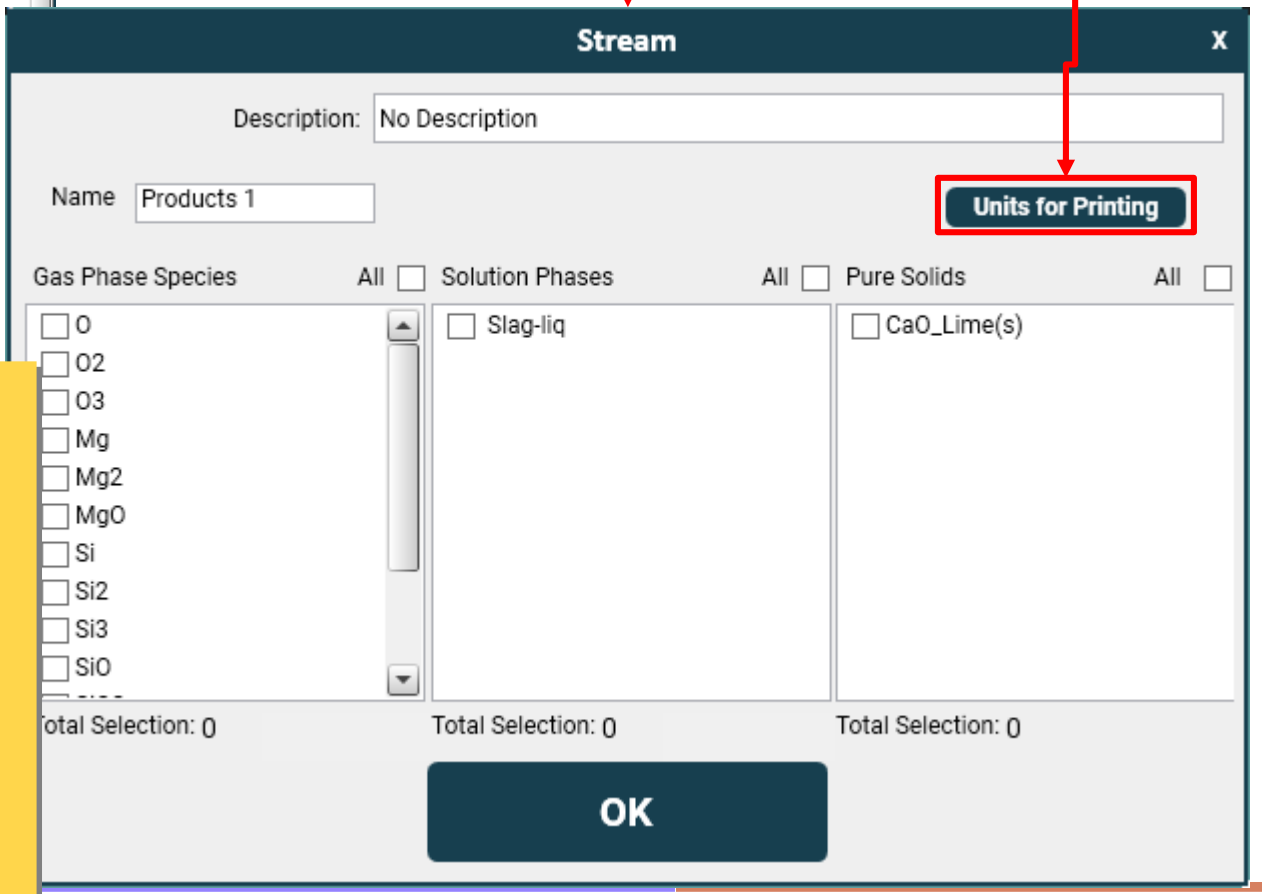


- The outgoing streams do not affect the Equilib calculations
- The phase selection of the reaction products is defined exclusively in the Equilib module, and is not affected by the presence and phase selection in the outgoing streams connected to the Equilib module
- The function of the outgoing streams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

Equilib Module – Outgoing streams (reaction products)



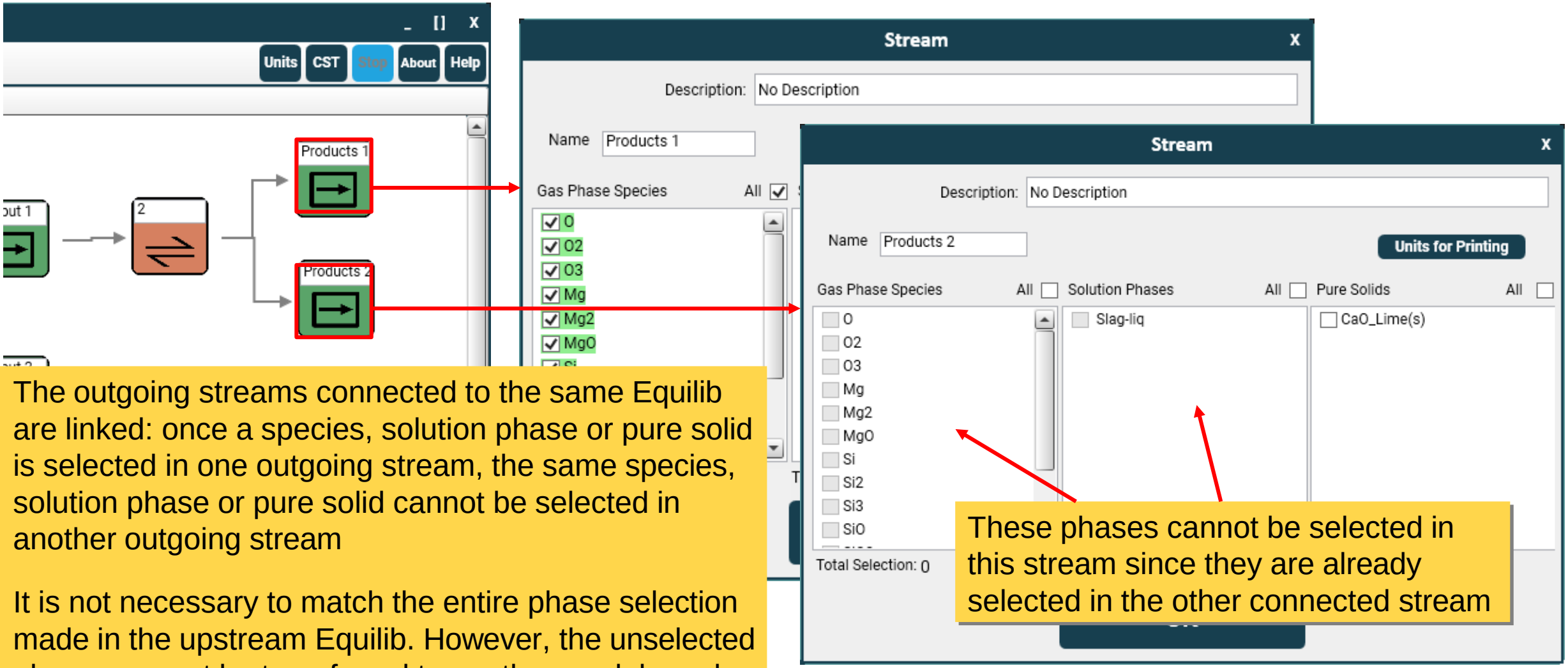
[Change the local units](#) when printing the content of this stream in its Excel worksheet



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)

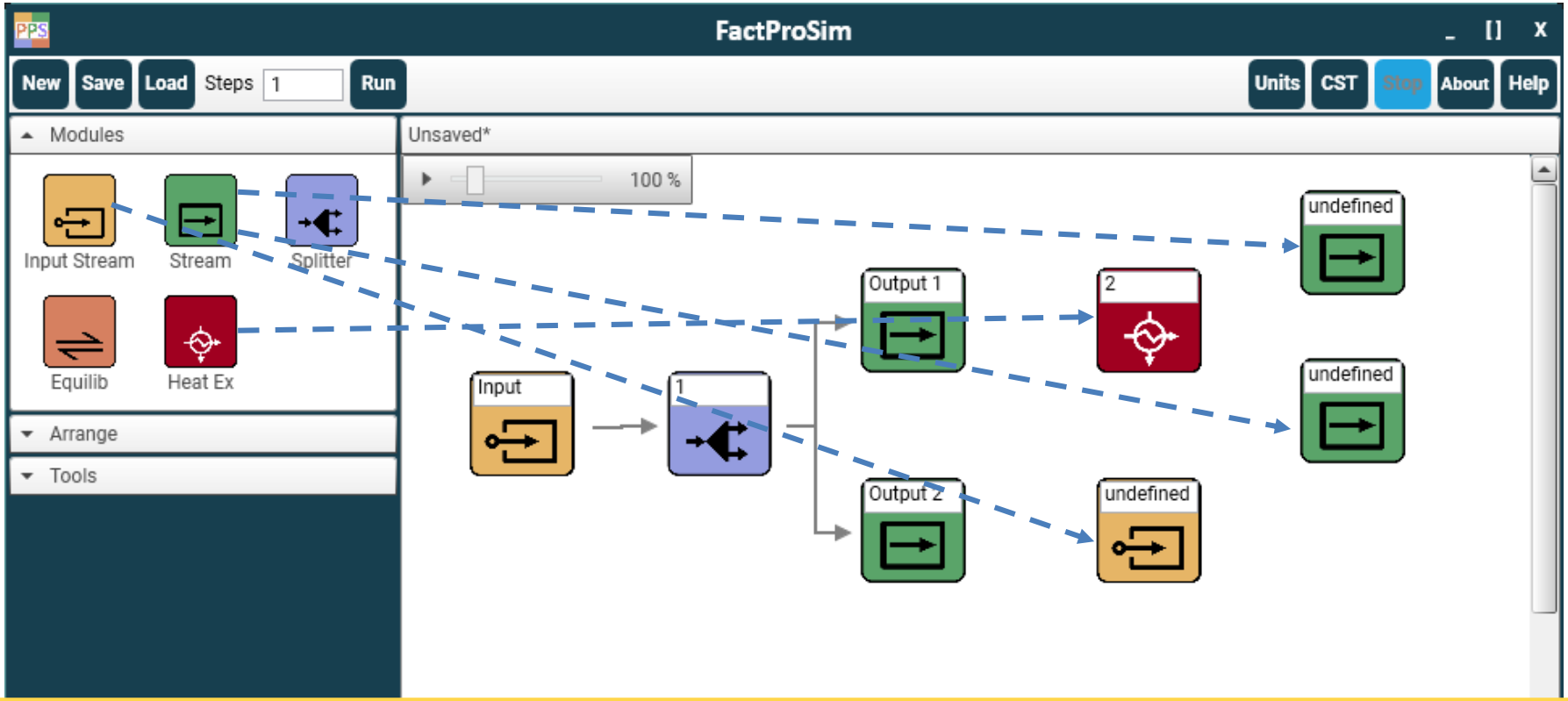


- The outgoing streams connected to the same Equilib are linked: once a species, solution phase or pure solid is selected in one outgoing stream, the same species, solution phase or pure solid cannot be selected in another outgoing stream
- It is not necessary to match the entire phase selection made 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

- 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)

Add Heat Exchanger and reactant streams in the diagram

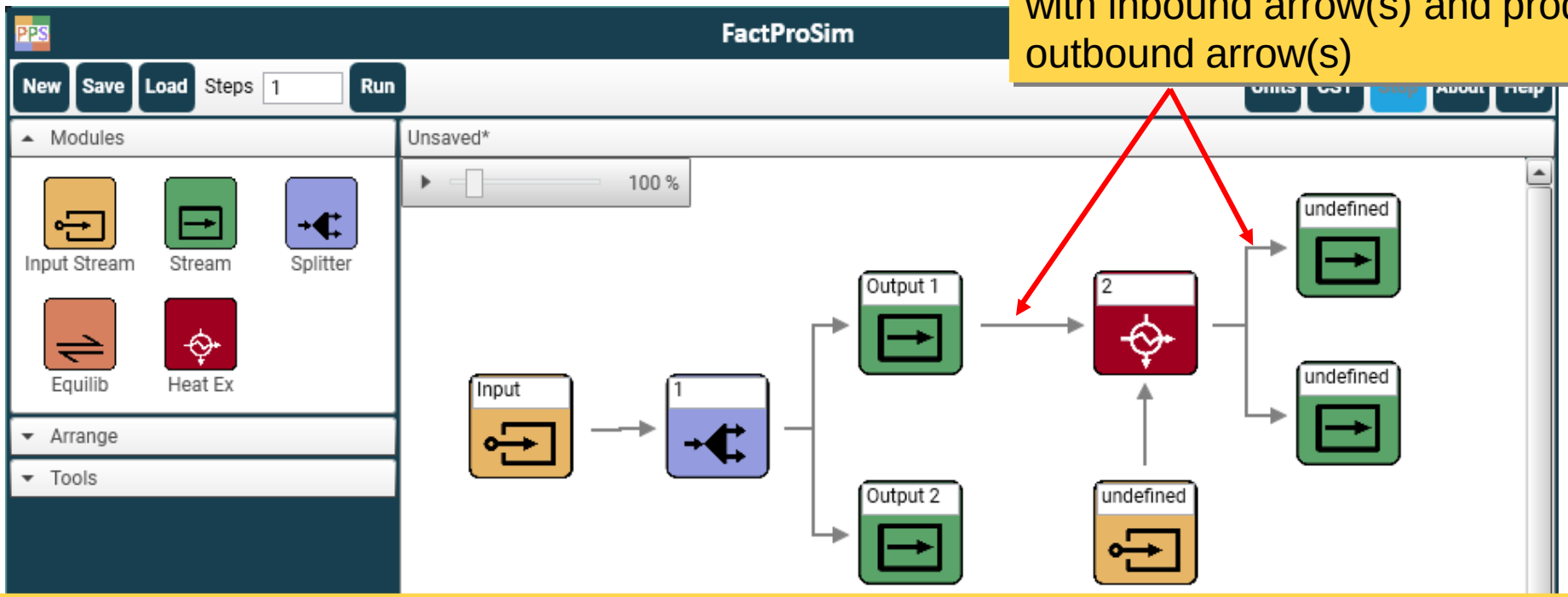


A Heat Exchanger allows to perform heat exchange between two reactant stream(s) and conditions set inside the module

- 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

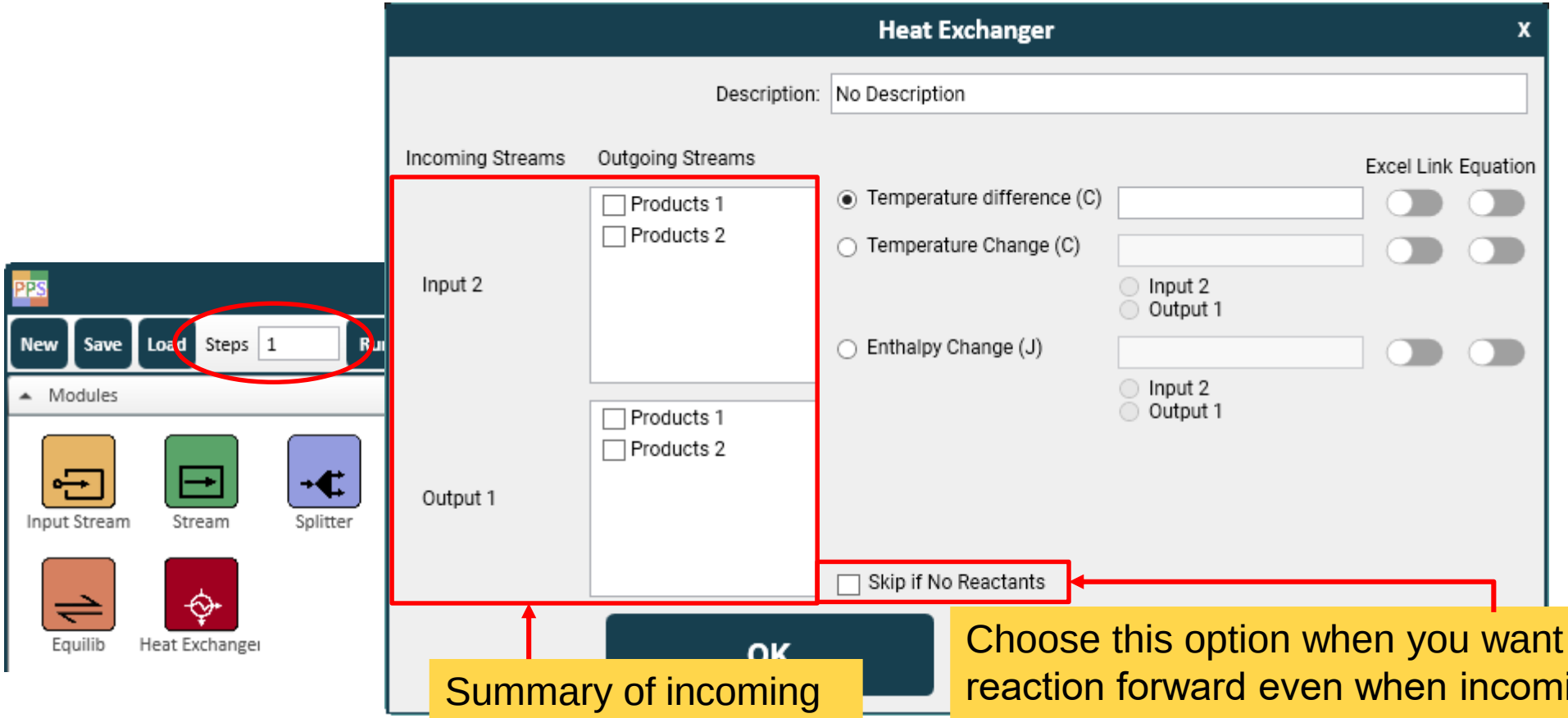
Add Heat Exchanger and reactant streams in the diagram

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

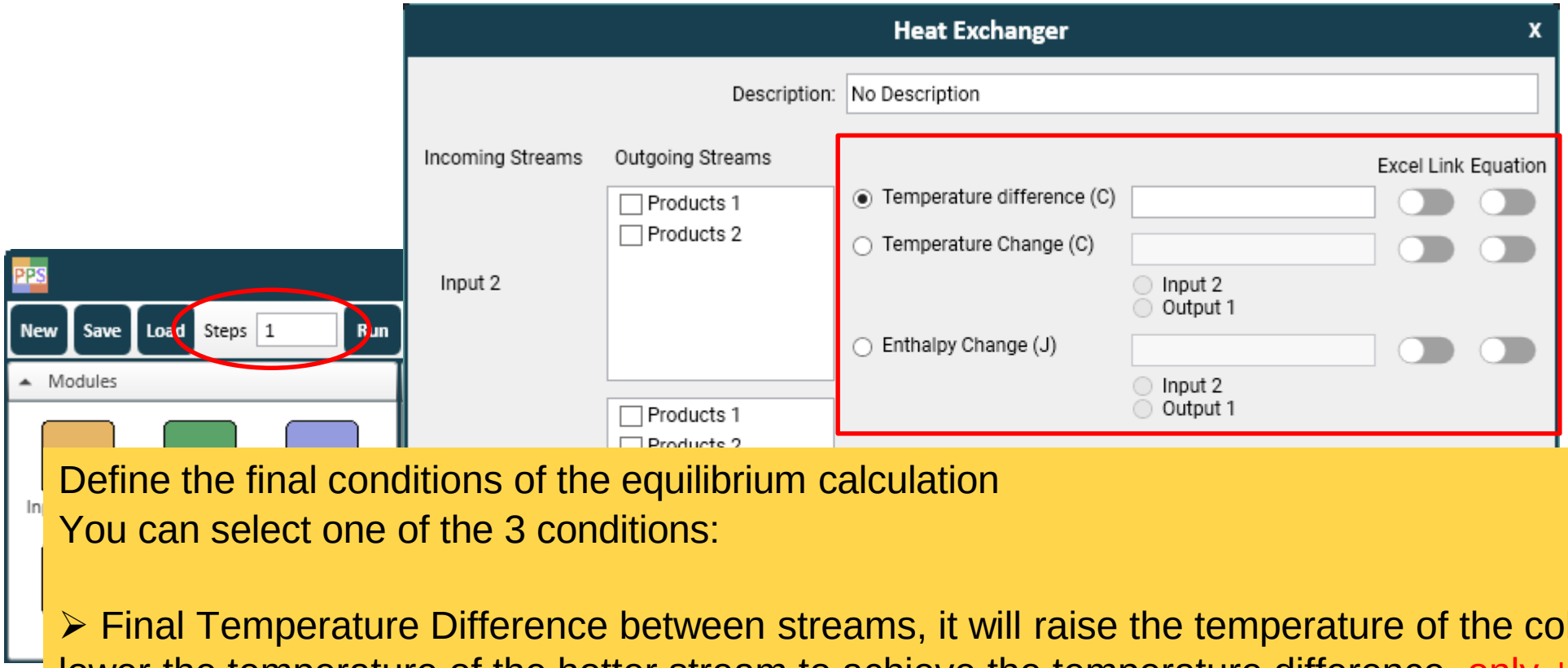


Summary of incoming and outgoing streams

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

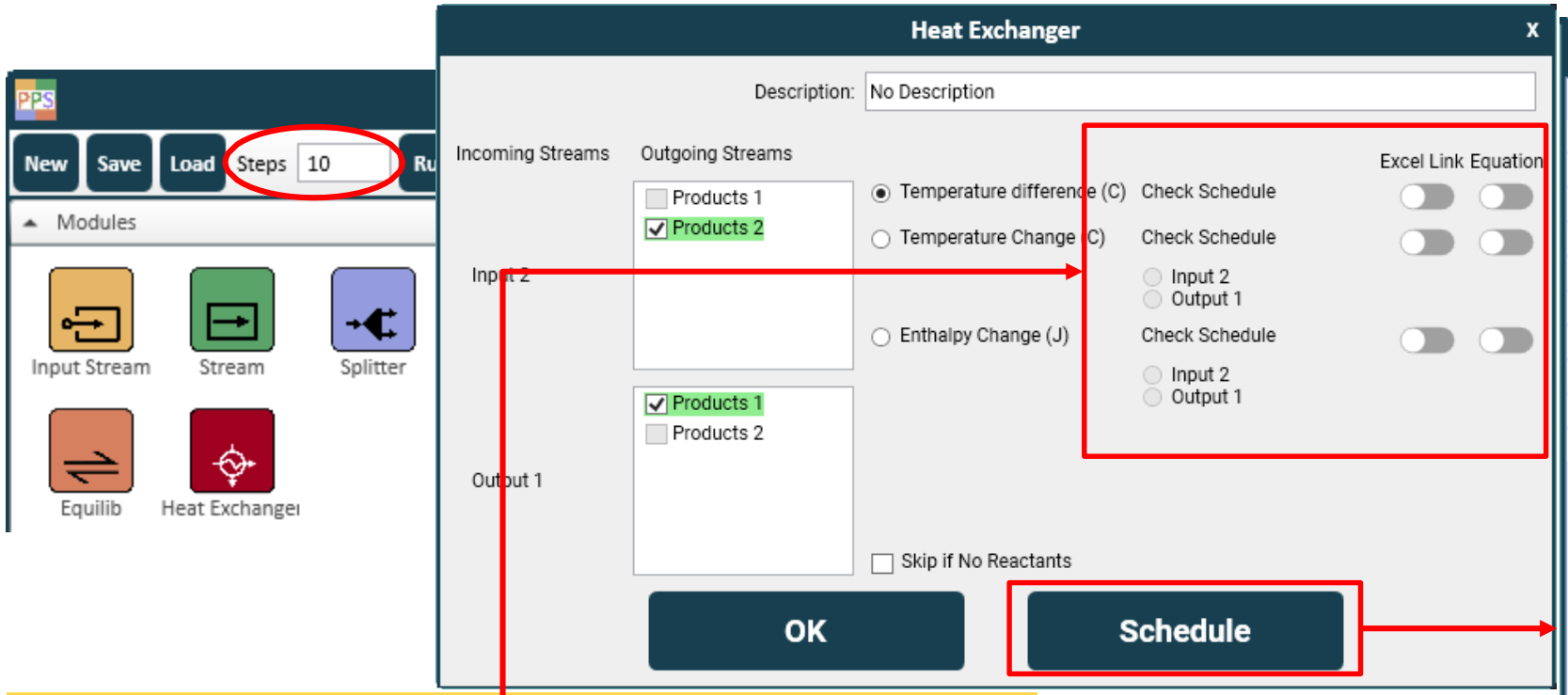
Heat Exchanger Module – Manual entry, 1 step

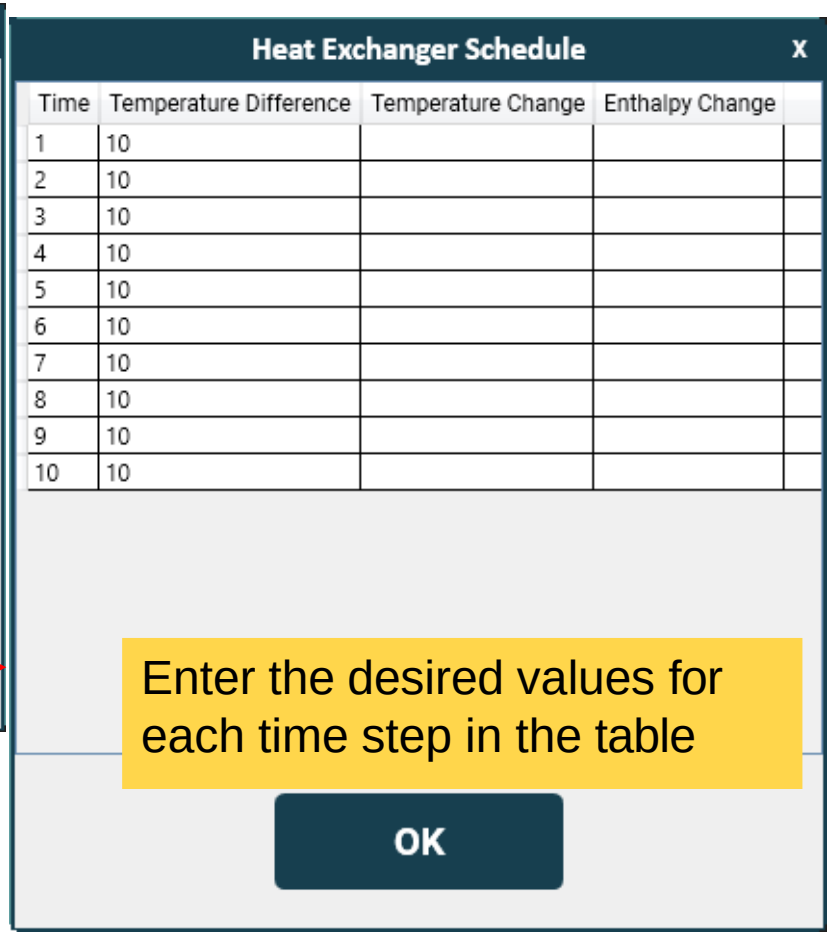


Define the final conditions of the equilibrium calculation
You can select one of the 3 conditions:

- 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



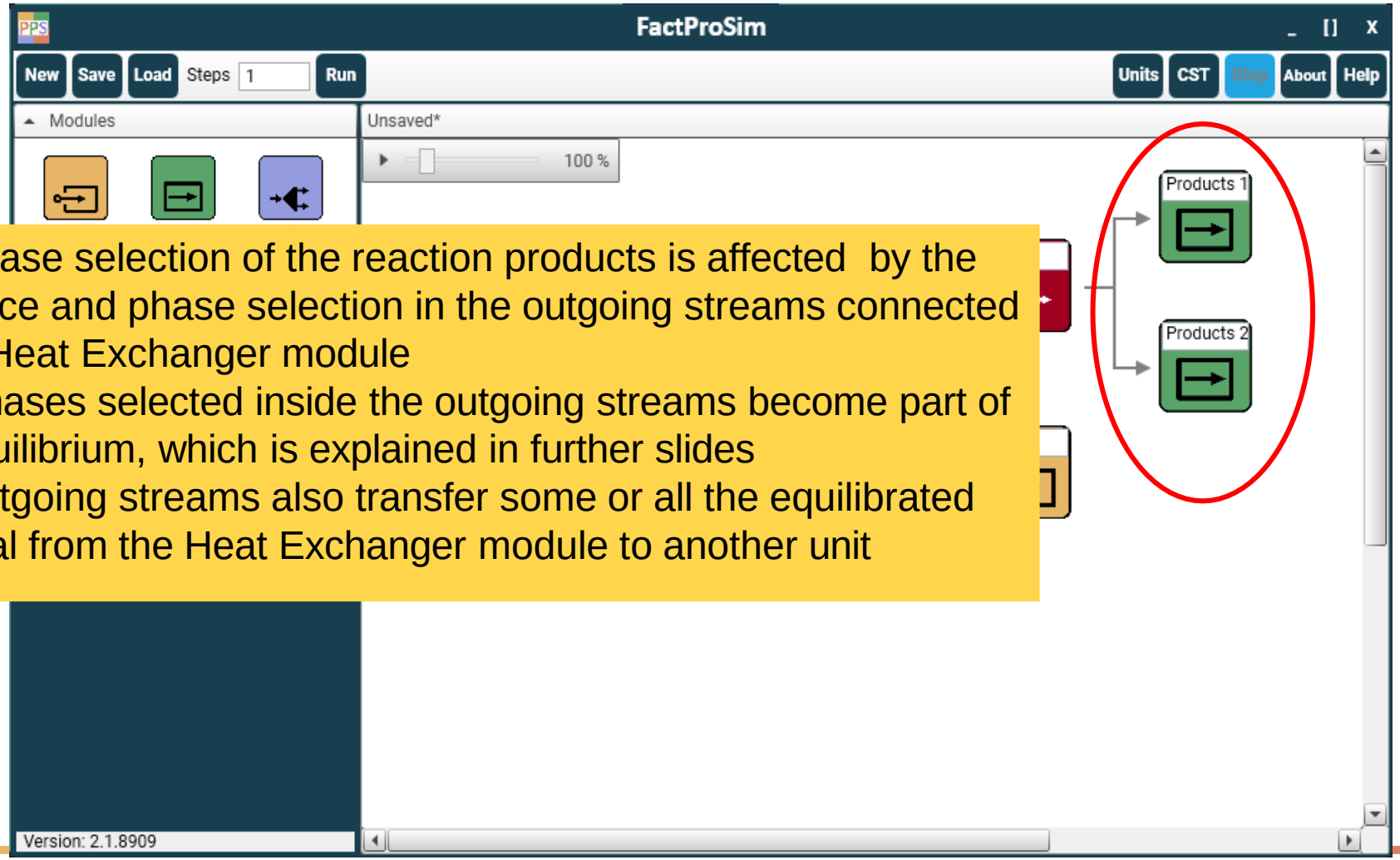


When more than 1 step is defined in the toolbar, different values can be used at each step

A schedule is needed to enter these values

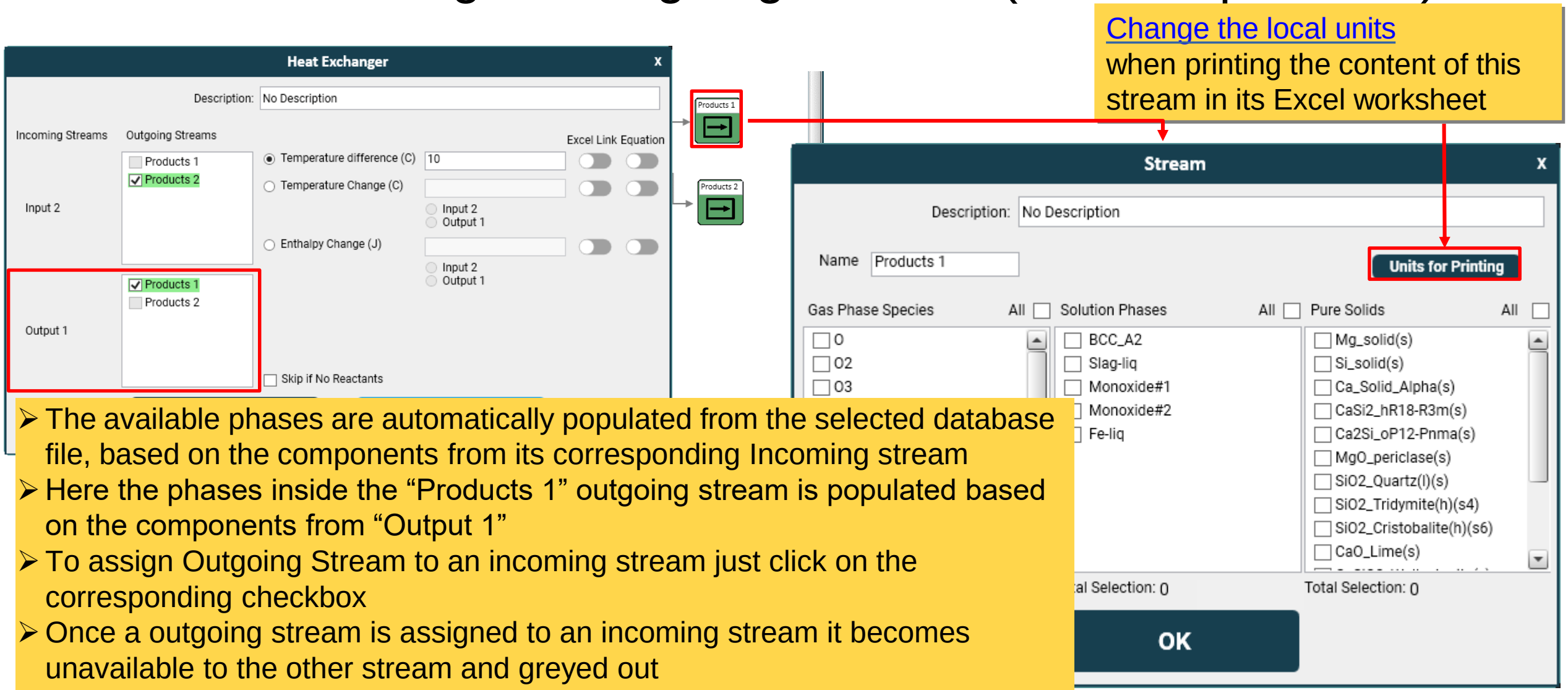
The Schedule button becomes available at the bottom of the module

Heat Exchanger– Outgoing streams (reaction products)



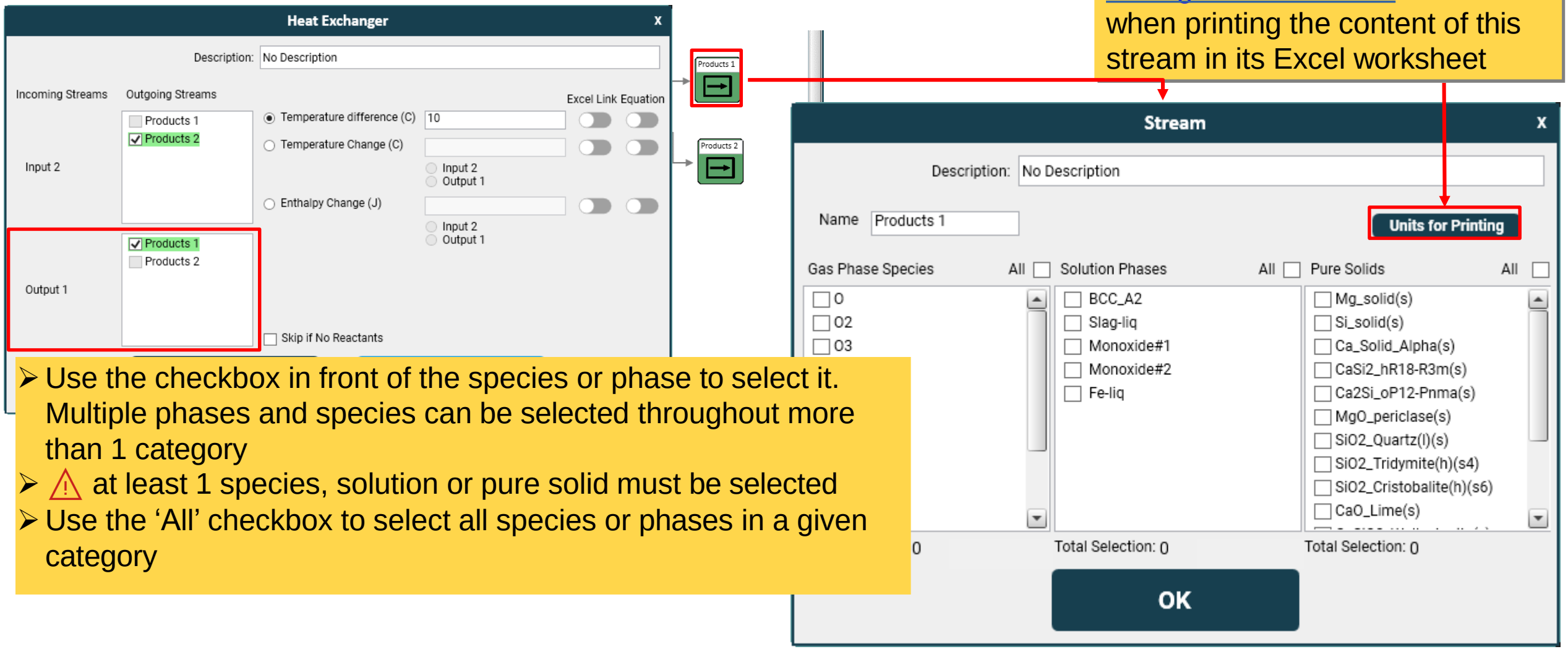
- The phase selection of the reaction products is affected by the presence and phase selection in the outgoing streams connected to the Heat Exchanger module
- The Phases selected inside the outgoing streams become part of the Equilibrium, which is explained in further slides
- The outgoing streams also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

Heat Exchanger– Outgoing streams (reaction products)



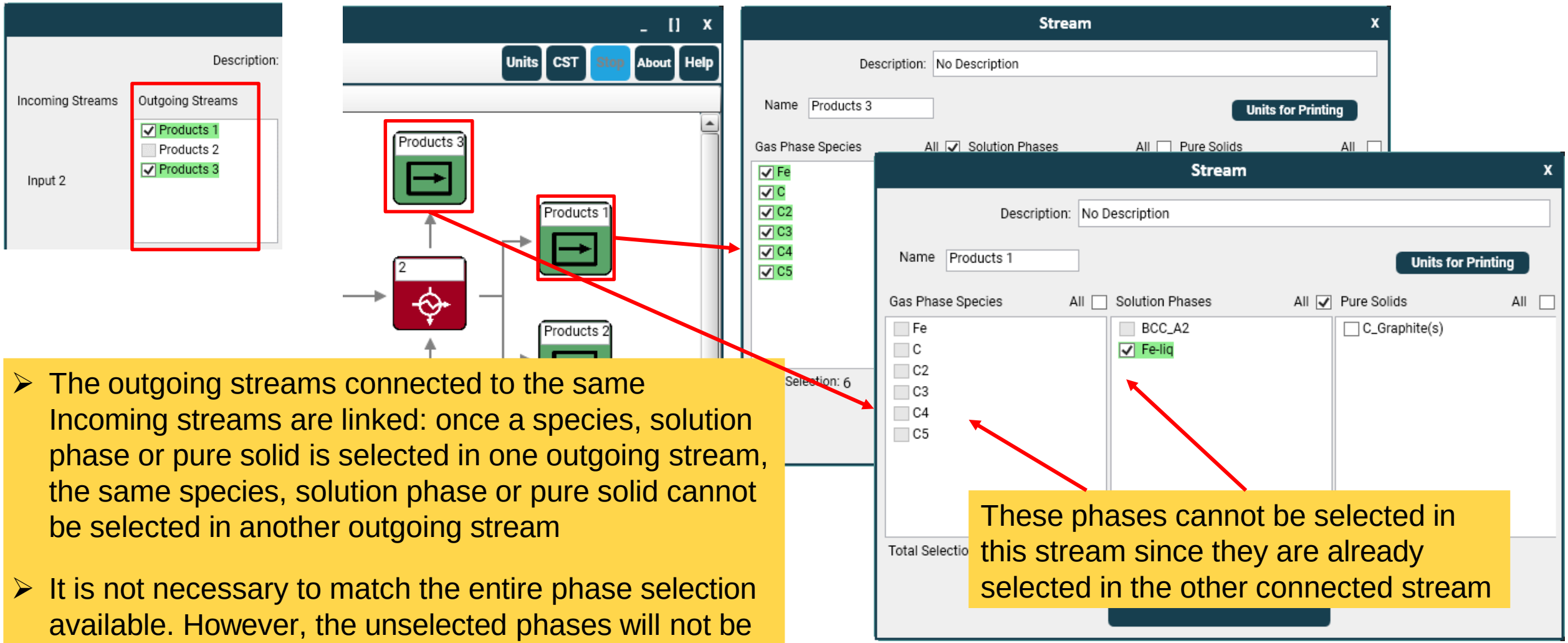
- The available phases are automatically populated from the selected database file, based on the components from its corresponding Incoming stream
- Here the phases inside the “Products 1” outgoing stream is populated based on the components from “Output 1”
- To assign Outgoing Stream to an incoming 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)



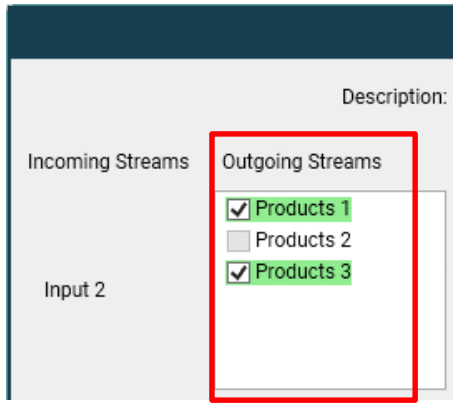
- Use the checkbox in front of the species or phase to select it. Multiple phases and species can be selected throughout more than 1 category
- ⚠ at least 1 species, solution or pure solid must be selected
- Use the ‘All’ checkbox to select all species or phases in a given category

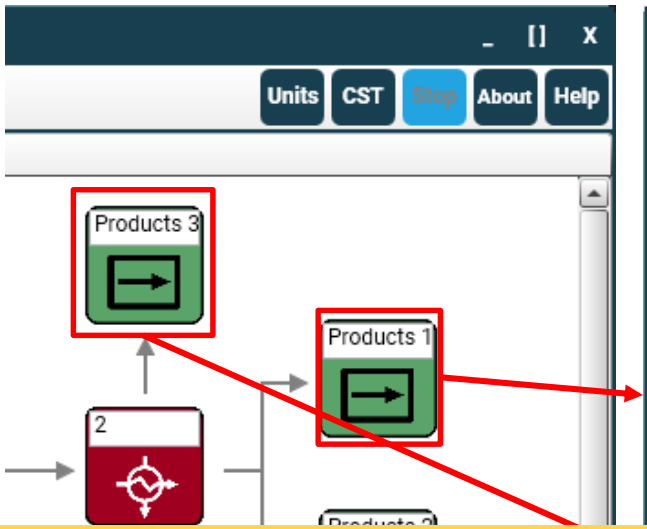
Heat Exchanger– Outgoing streams (reaction products)

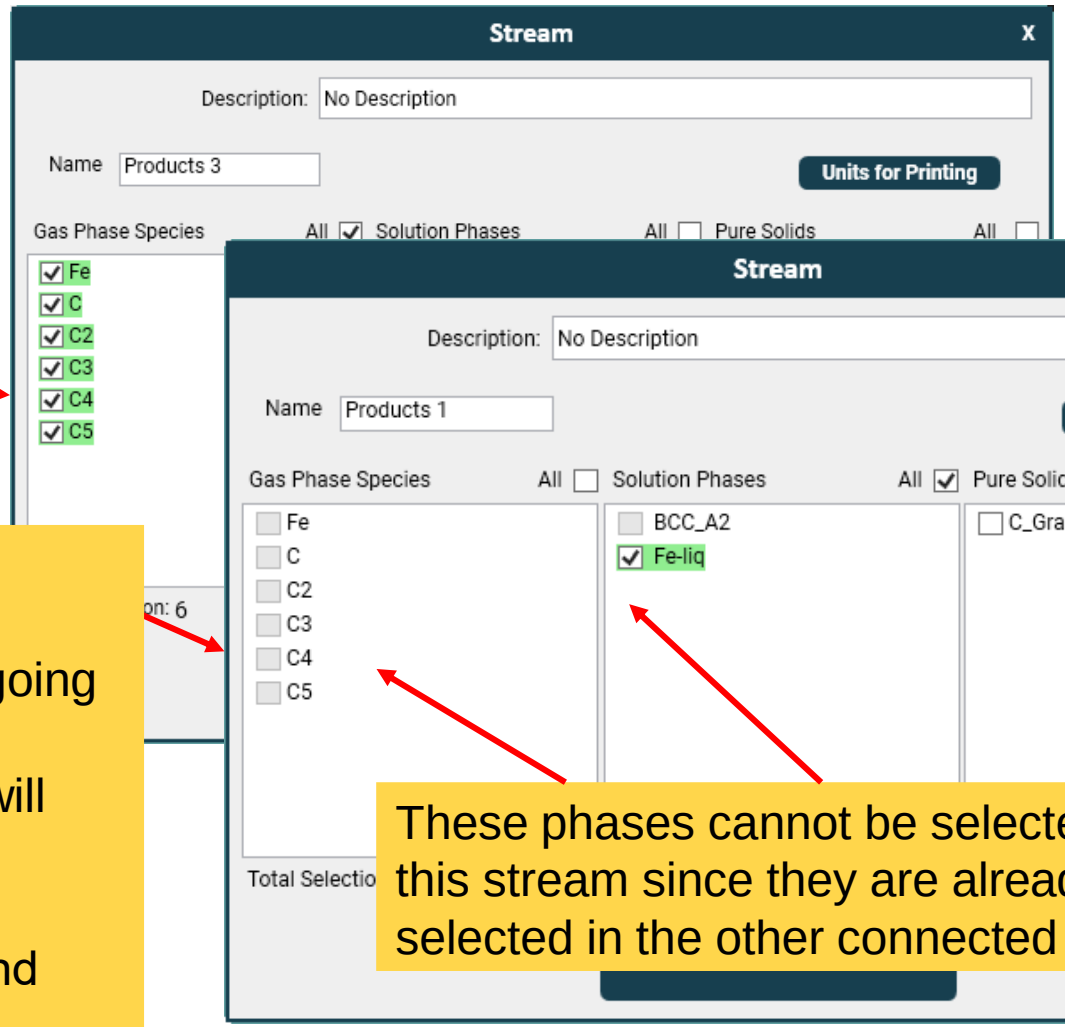


- The outgoing streams connected to the same Incoming streams are linked: once a species, solution phase or pure solid is selected in one outgoing stream, the same species, solution phase or pure solid cannot be selected in another outgoing stream
- It is not necessary to match the entire phase selection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

Heat Exchanger– Outgoing streams (reaction products)







Phase Selection:

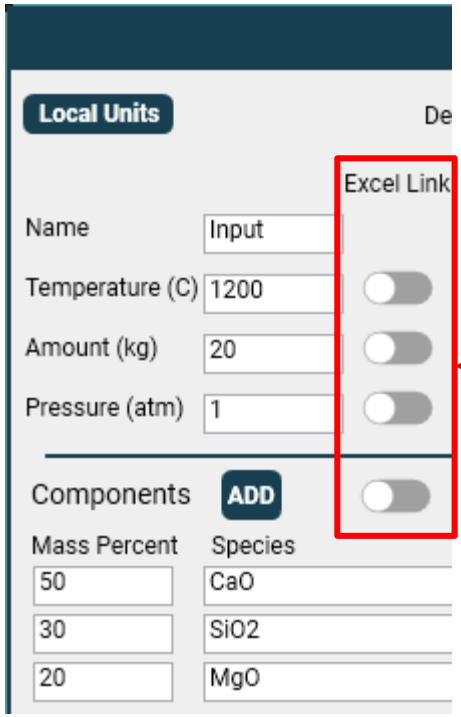
- The final Equilibrium state of the incoming stream is defined by the phases selected inside its linked outgoing streams
- The equilibrium calculation of the incoming stream will add all the phases in all the outgoing stream and incorporate them
- Here the Gas Phase and Fe-liq from “Products 1” and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

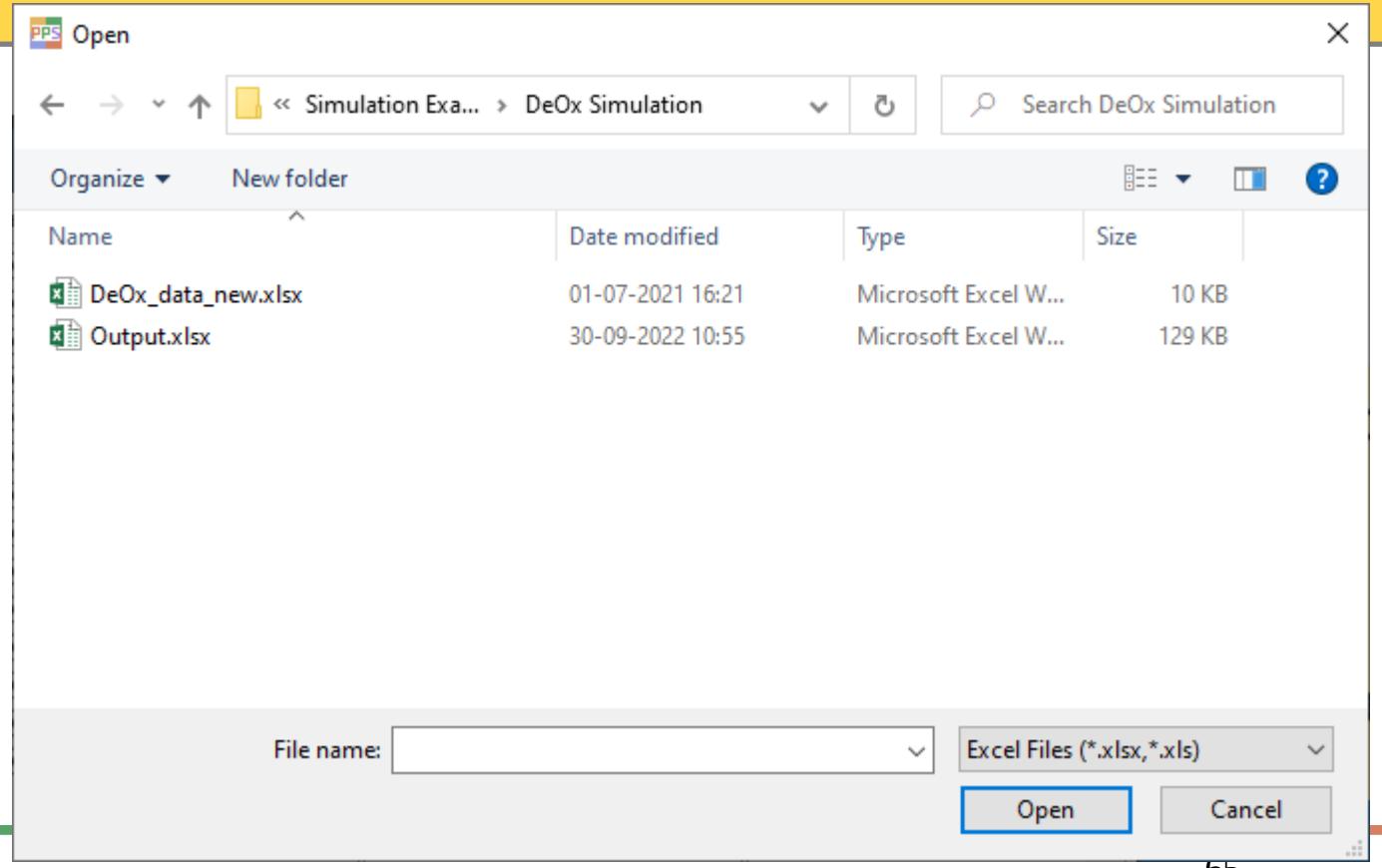
Description of the program

- 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**
- 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

Using Excel links – single field



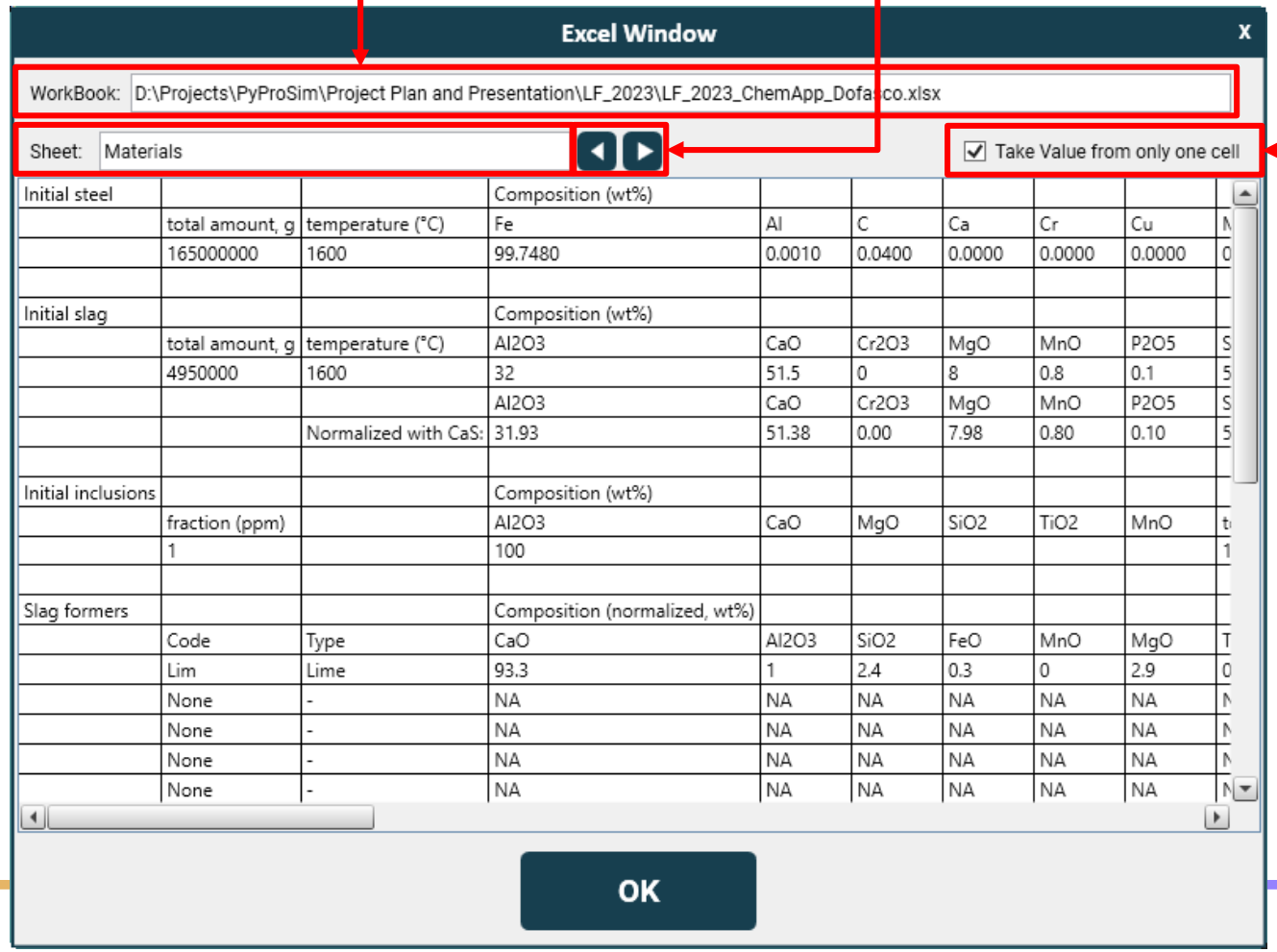
- Some fields can be connected to cells in an Excel worksheet using the Excel Link option
- To activate the link for a given field, click the toggle button next to the field
- A browse window opens. Locate and select the Excel file on your computer and click Open



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)

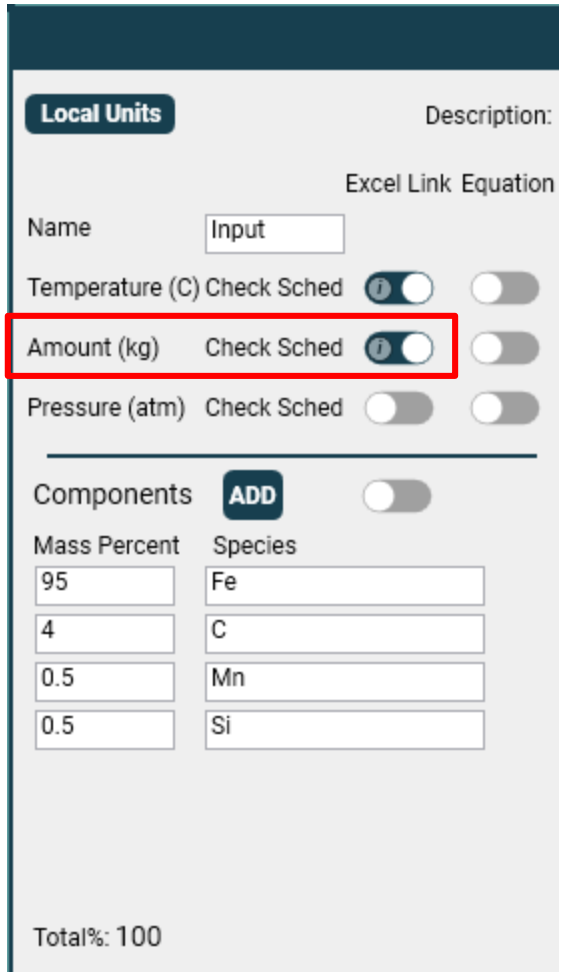


Initial steel			Composition (wt%)						
	total amount, g	temperature (°C)	Fe	Al	C	Ca	Cr	Cu	N
	165000000	1600	99.7480	0.0010	0.0400	0.0000	0.0000	0.0000	0
Initial slag			Composition (wt%)						
	total amount, g	temperature (°C)	Al2O3	CaO	Cr2O3	MgO	MnO	P2O5	S
	4950000	1600	32	51.5	0	8	0.8	0.1	5
			Al2O3	CaO	Cr2O3	MgO	MnO	P2O5	S
		Normalized with CaS:	31.93	51.38	0.00	7.98	0.80	0.10	5
Initial inclusions			Composition (wt%)						
	fraction (ppm)		Al2O3	CaO	MgO	SiO2	TiO2	MnO	t
	1		100						1
Slag formers			Composition (normalized, wt%)						
	Code	Type	CaO	Al2O3	SiO2	FeO	MnO	MgO	T
	Lim	Lime	93.3	1	2.4	0.3	0	2.9	0
	None	-	NA	NA	NA	NA	NA	NA	N
	None	-	NA	NA	NA	NA	NA	NA	N
	None	-	NA	NA	NA	NA	NA	NA	N
	None	-	NA	NA	NA	NA	NA	NA	N

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

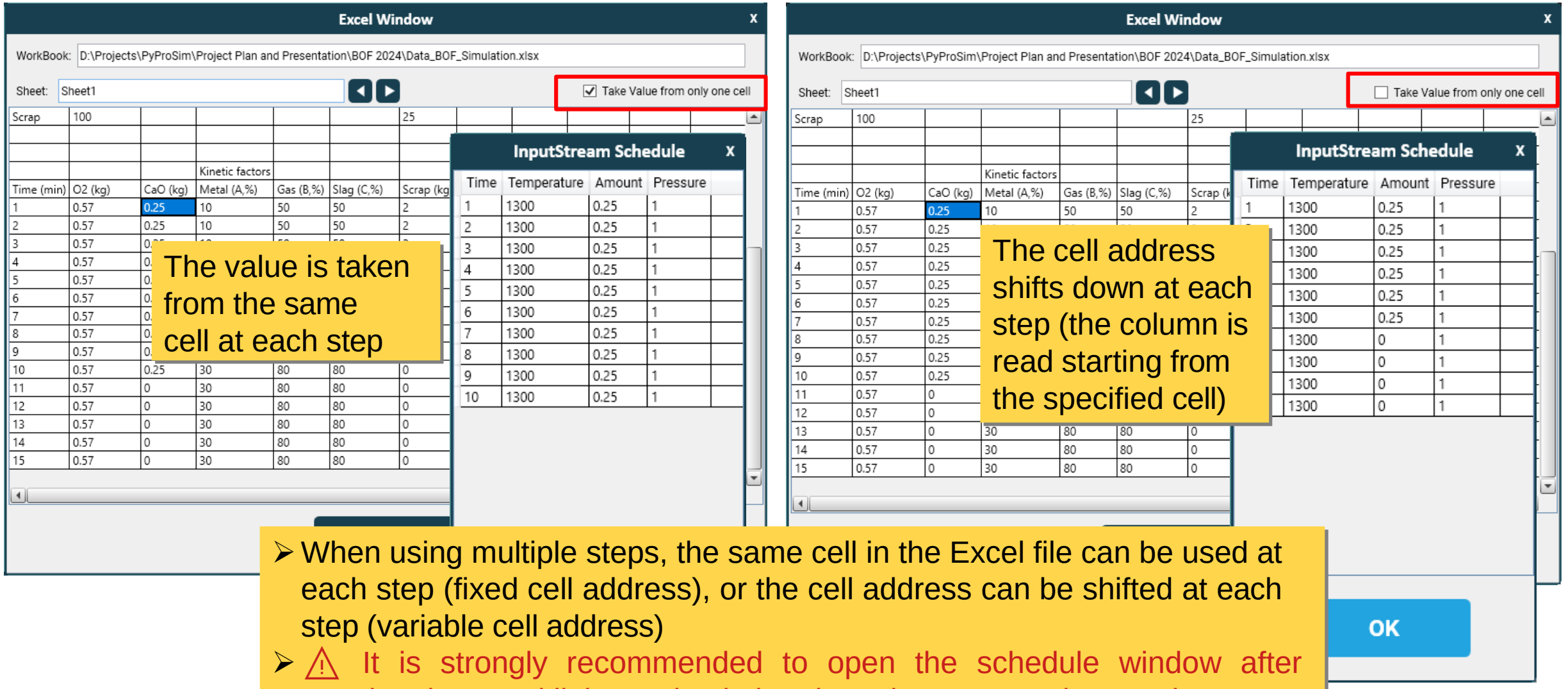
- An Excel window opens with the content of each worksheet in the selected Excel file (without formulas and formatting) in a table format
- Click in the desired cell to indicate which cell address to take the value from
- At the right-hand corner of the window, select the checkbox to indicate whether 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)



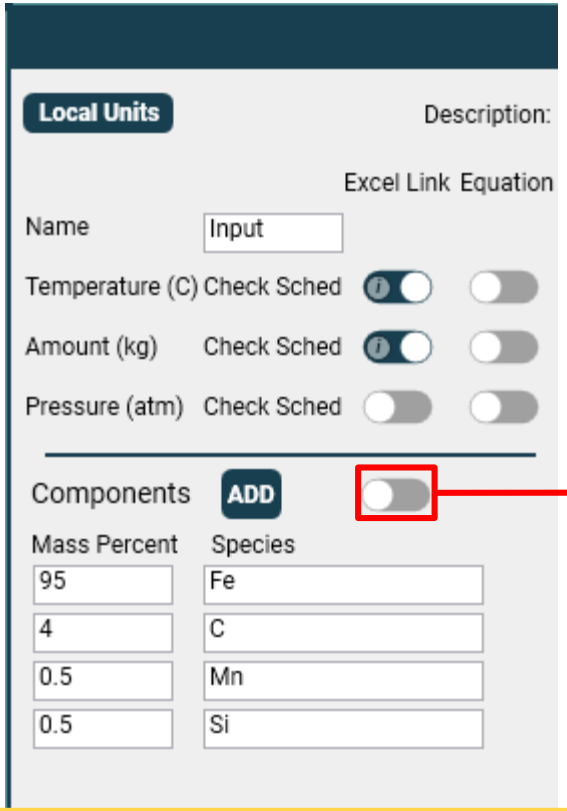
- When the value from the Excel cell is successfully read, the value is entered in the field and becomes non-editable. The toggle button is on (dark background)
- When the Excel Link is on, the value of the field will be updated with the value stored at the cell address in the Excel file every time the 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

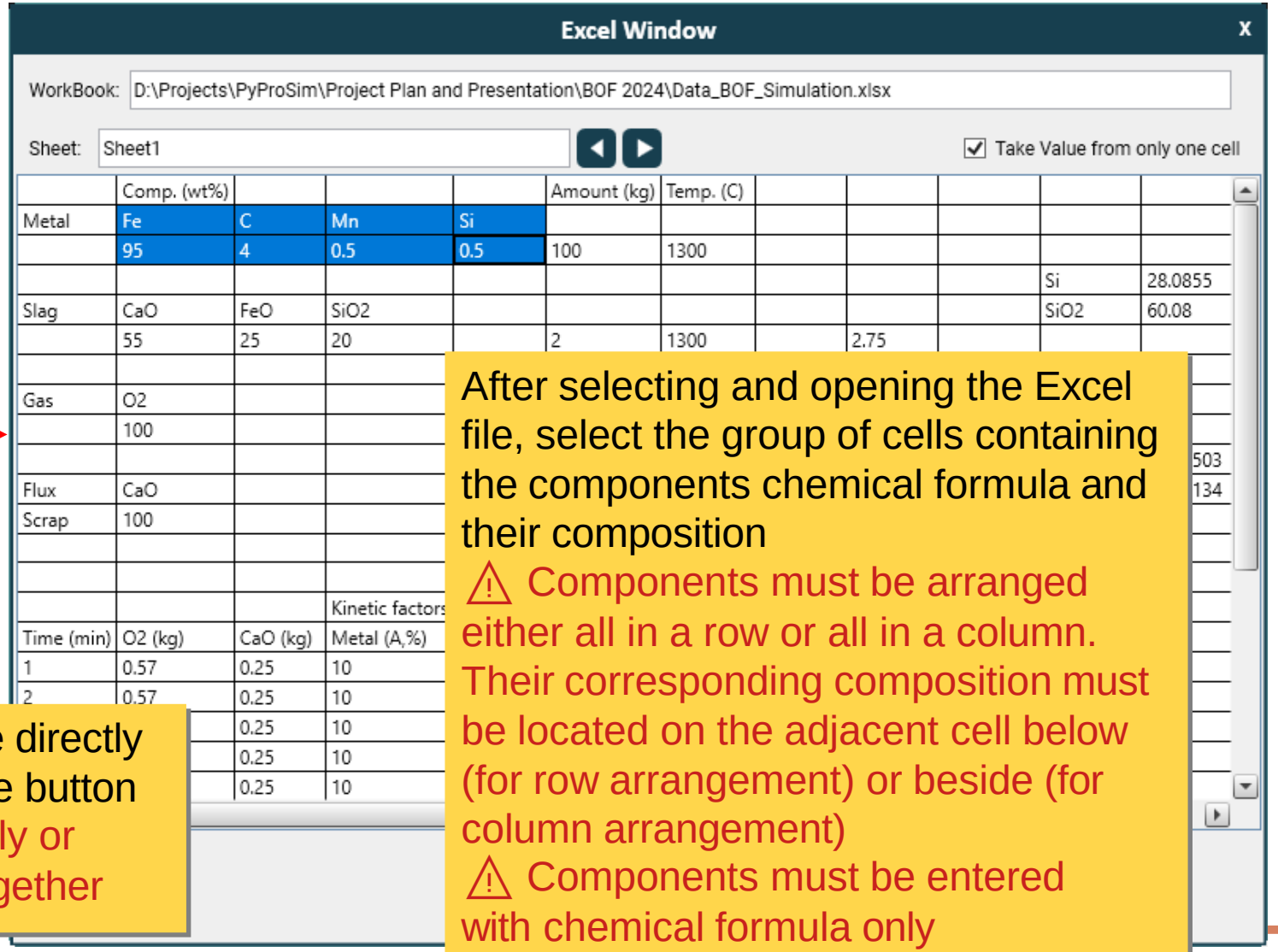
Using Excel links – fixed vs. variable cell address



- 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

Using Excel links – Entering components (Input Stream)





The components and their composition can be directly imported from Excel using the Excel link toggle button

⚠ components can be entered either manually or via the Excel Link, but both cannot be used together

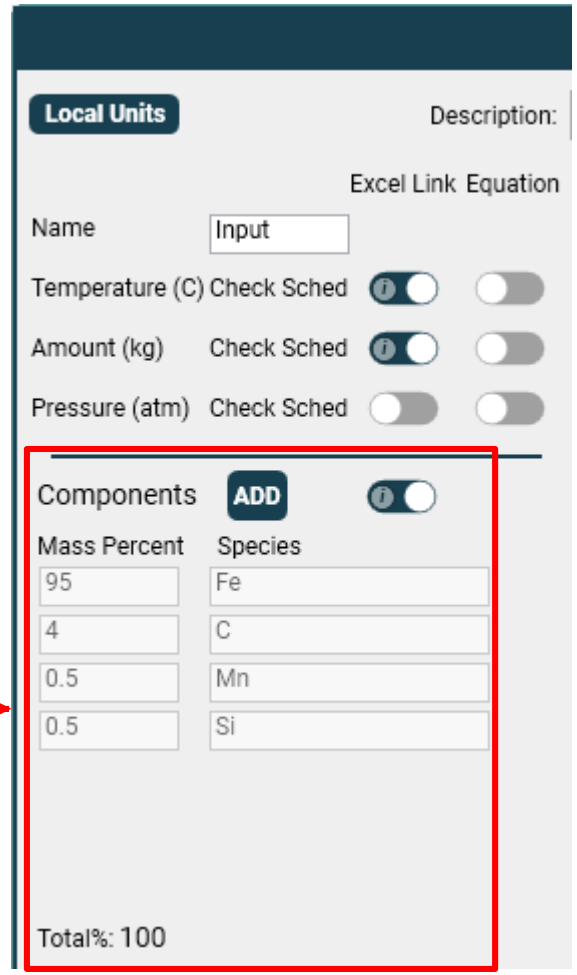
After selecting and opening the Excel file, select the group of cells containing the components chemical formula and their composition

⚠ Components must be arranged either all in a row or all in a column. Their corresponding composition must be located on the adjacent cell below (for row arrangement) or beside (for column arrangement)

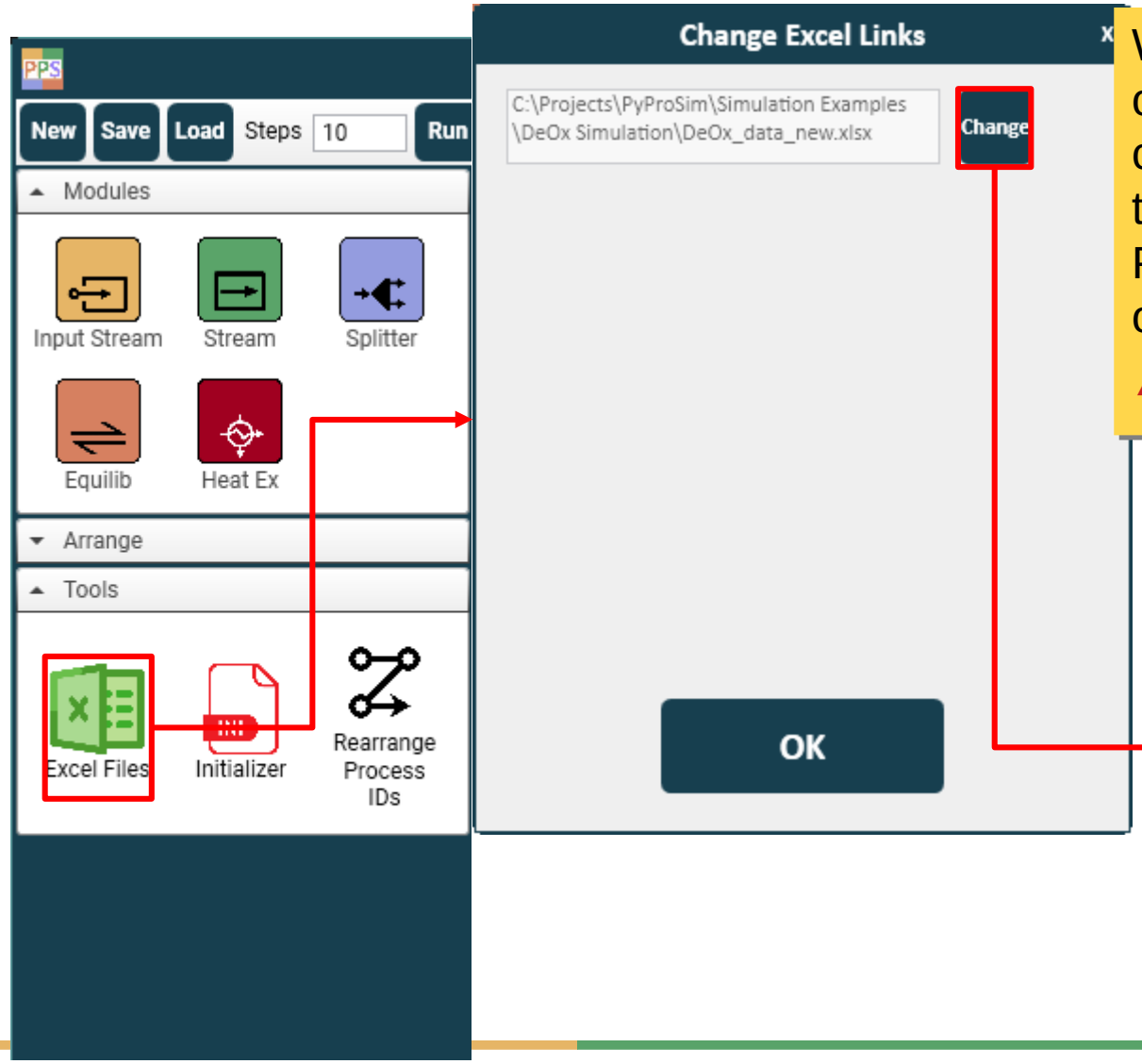
⚠ Components must be entered with chemical formula only

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



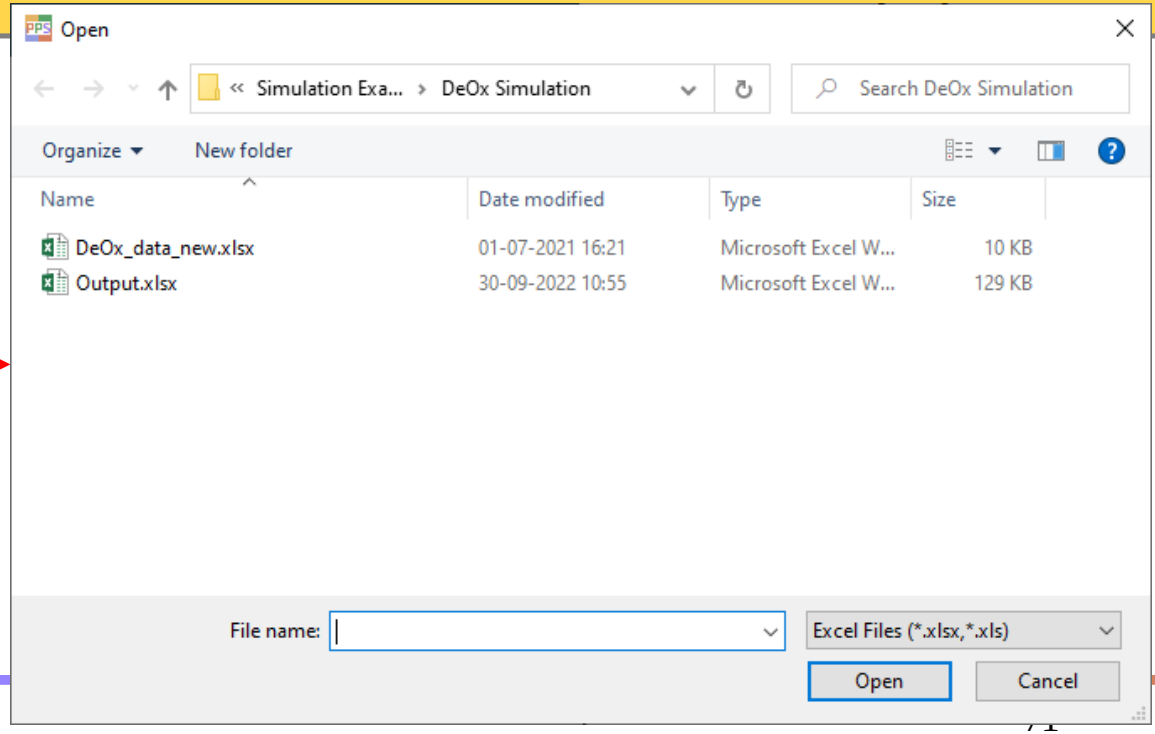
Using Excel links – Changing the Excel file(s)



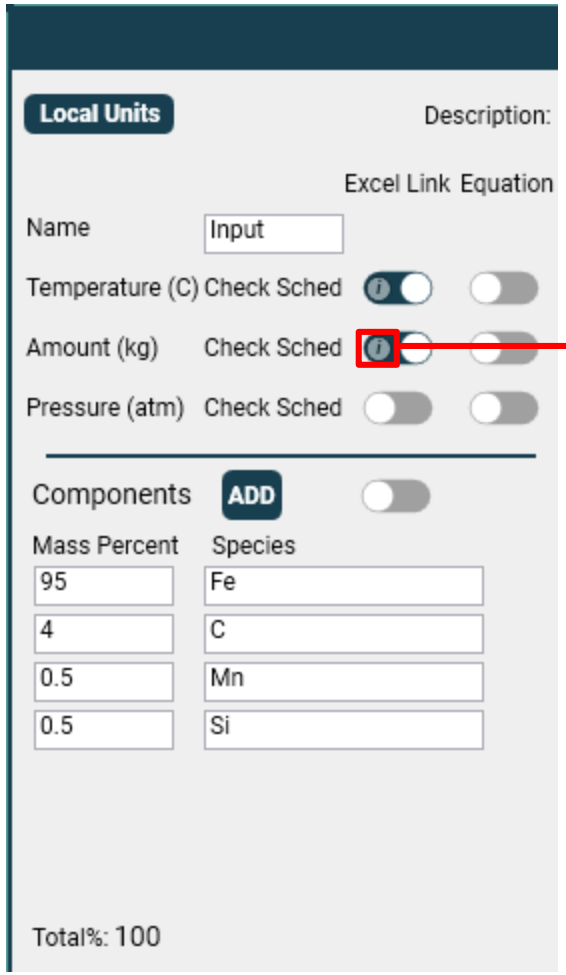
When using Excel links in modules, the name and location of the Excel source files is stored with the flowsheet. It can be viewed and changed using the Excel Files button in the Tools Panel

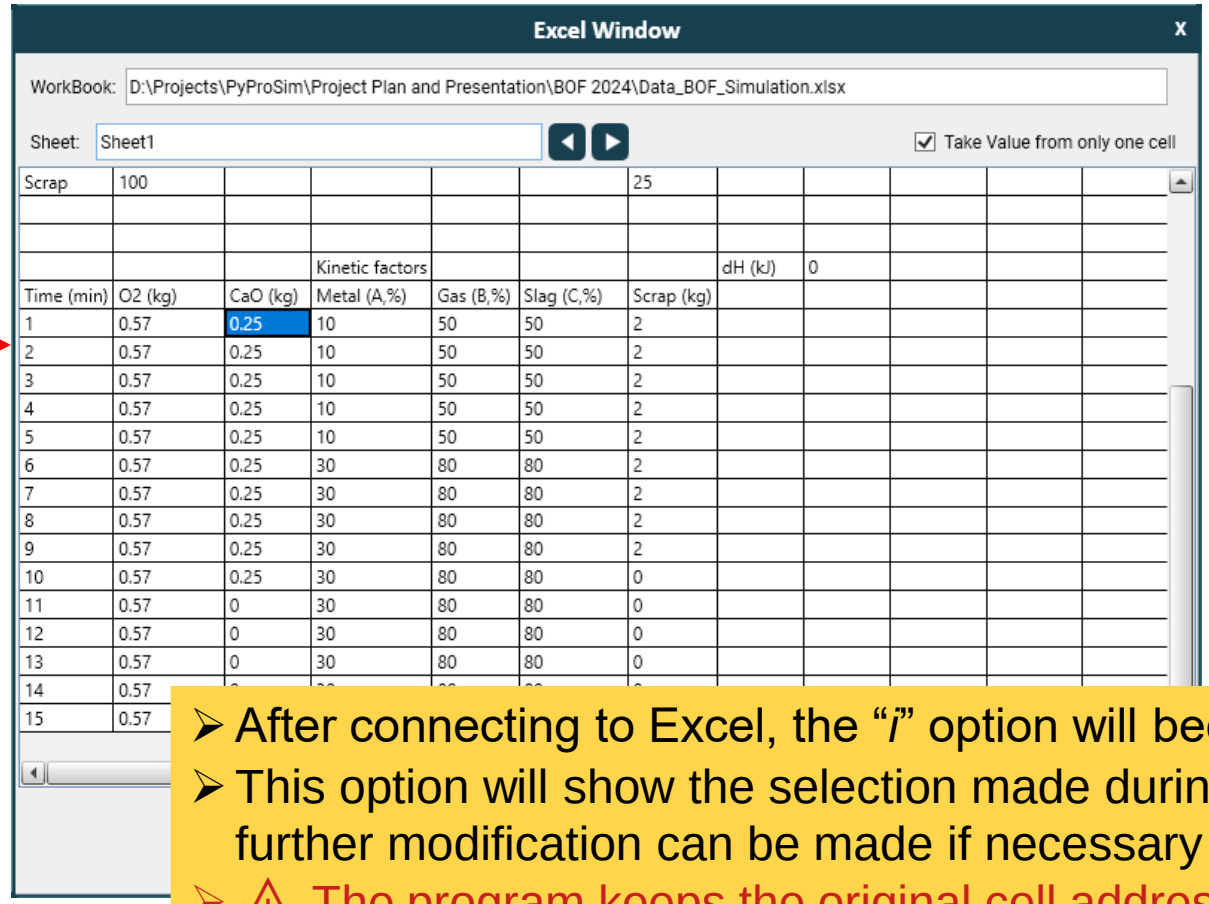
Press the Change button next to the Excel file path to open a browse window and select a different Excel file

⚠ Cell addresses provided in the modules are unchanged



Using Excel links – Reviewing the selection



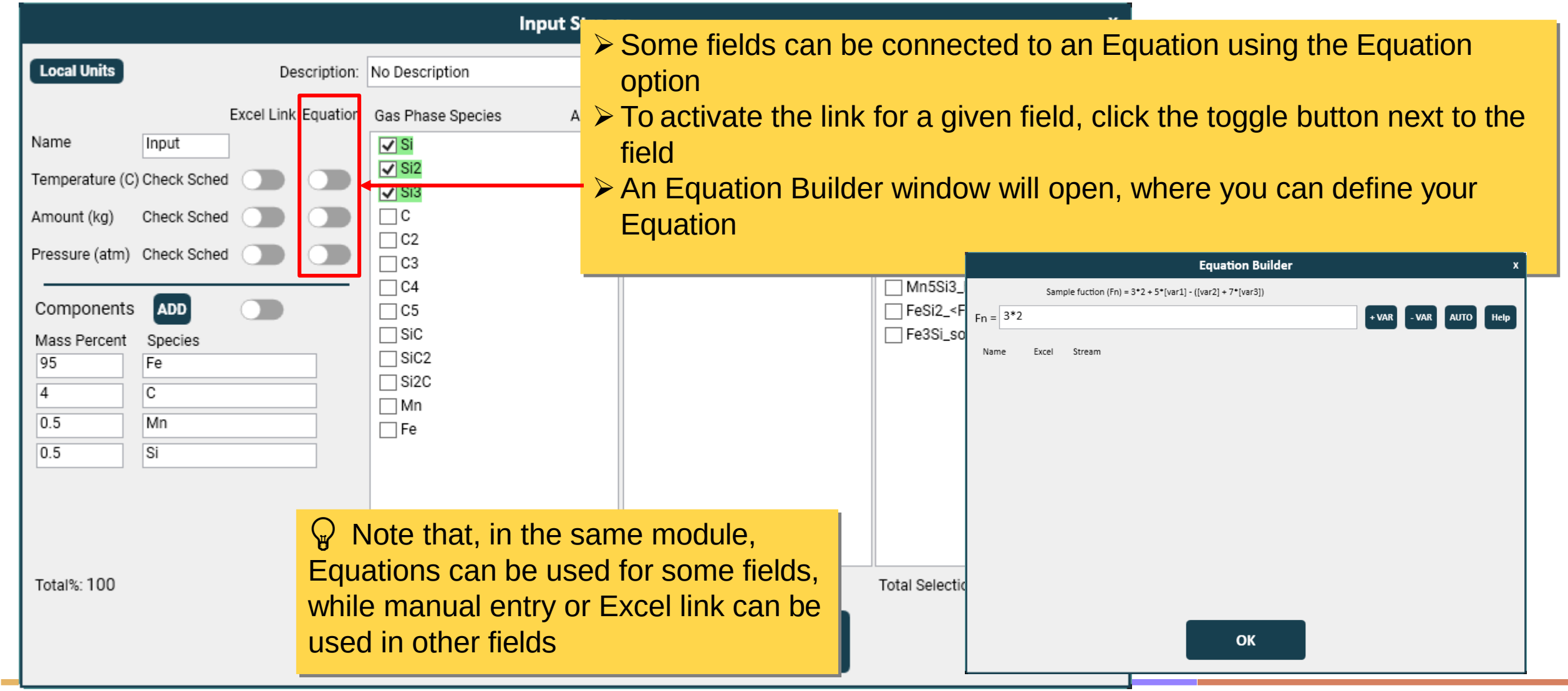


- After connecting to Excel, the "*i*" option will become active
- This option will show the selection made during connection and further modification can be made if necessary
- ⚠ The program keeps the original cell address: if the user inserts or deletes columns/rows, or moves the cell in the Excel 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
- 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

Using Equation

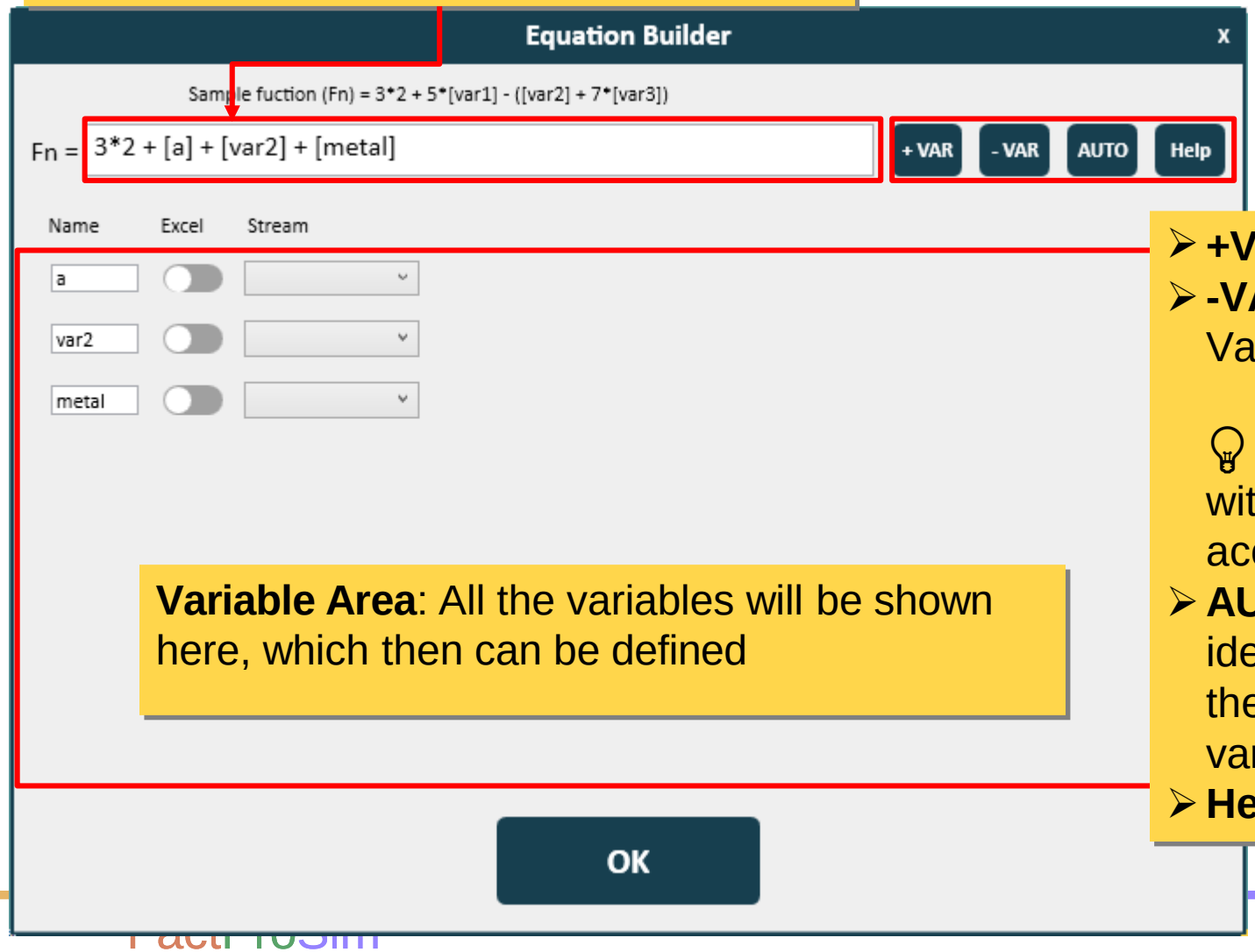


- Some fields can be connected to an Equation using the Equation option
- To activate the link for a given field, click the toggle button next to the field
- An Equation Builder window will open, where you can define your Equation

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

Using Equation

Equation Area: Write your equation here

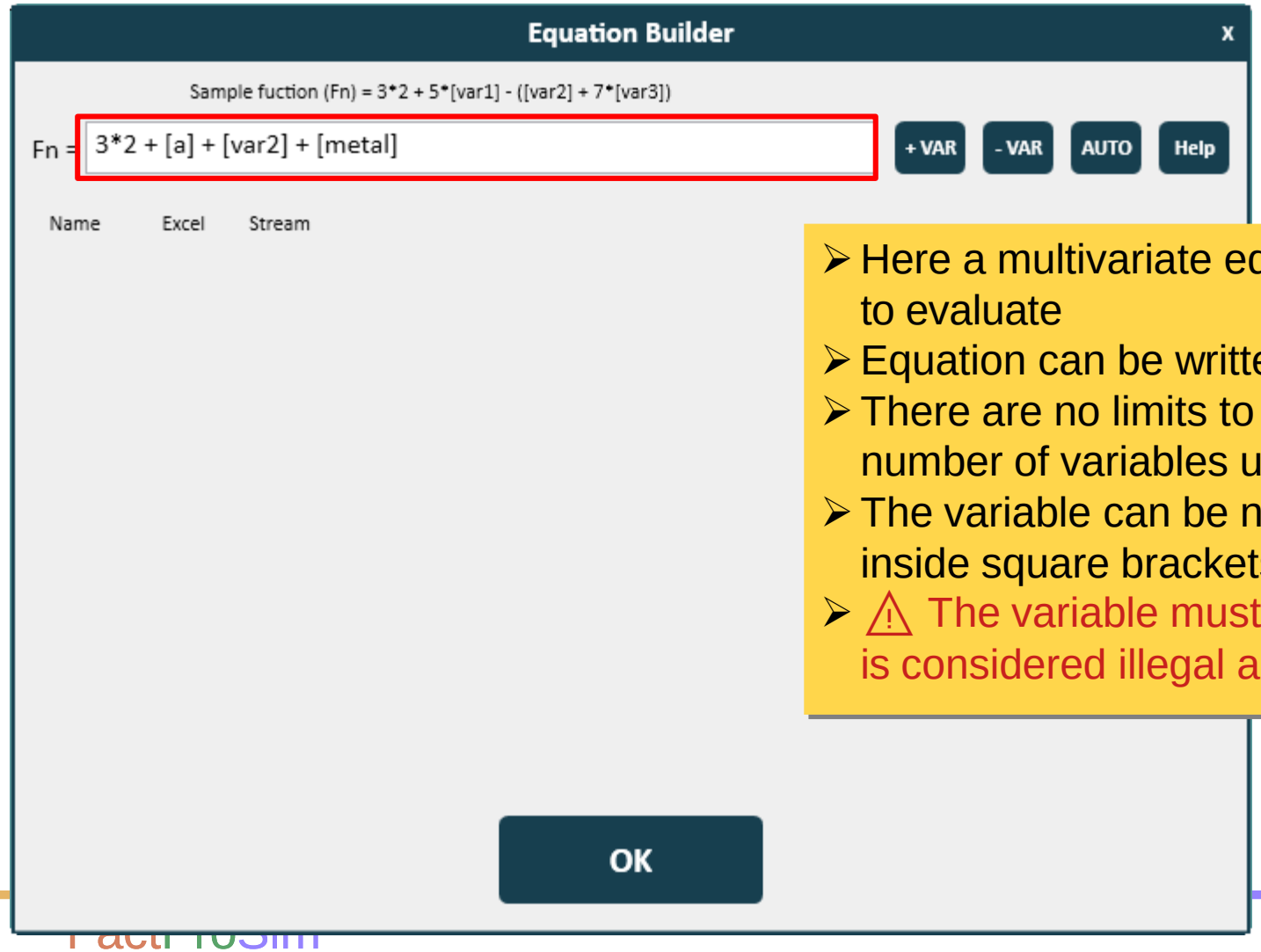


Variable Area: All the variables will be shown here, which then can be defined

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

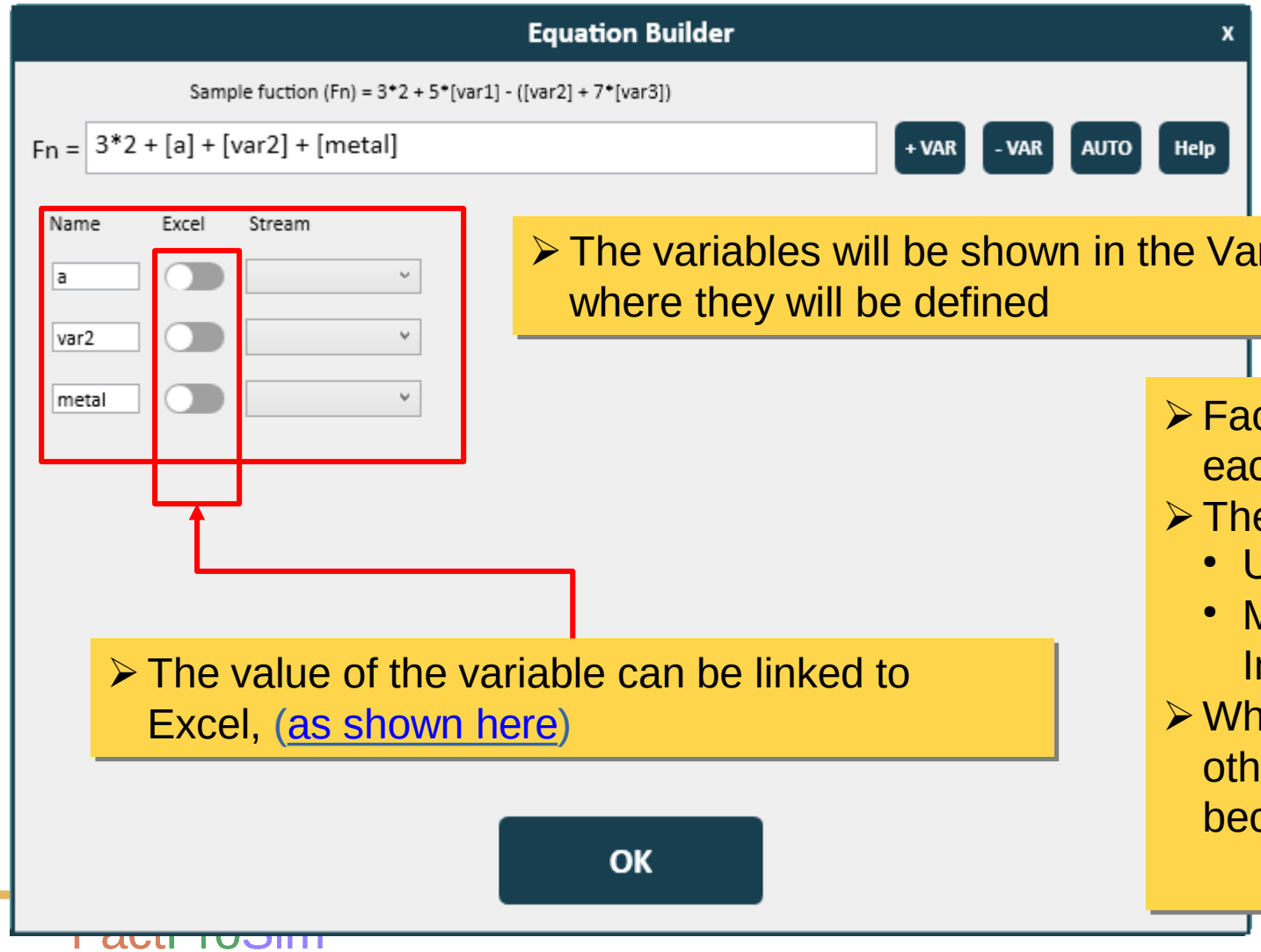
  These two options will only generate variables with generic name, user need to rewrite the name according to equation variables
- **AUTO** will read the equation in the *Equation Area*, identifies the written variables in the equation and then populate the *Variable Area* with corresponding variables
- **Help** will open this user manual

Using Equation: Equation Text



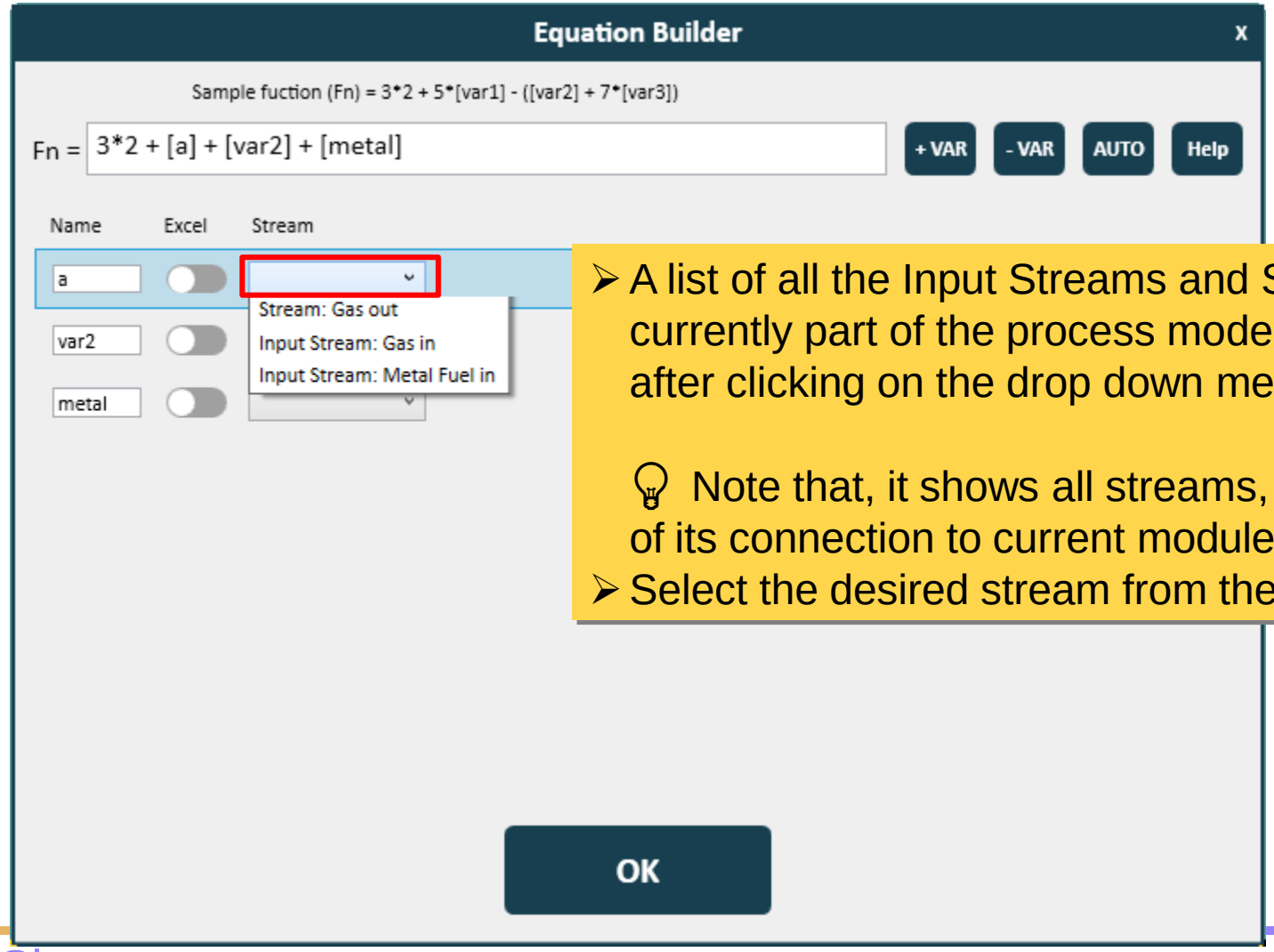
- Here a multivariate equation can be written for the FactProSim to evaluate
- Equation can be written in the form similar to Excel
- There are no limits to the length of the equation and the number of variables used
- The variable can be named anything as long as they are written inside square brackets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

Using Equation: Variable declarations



- The 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

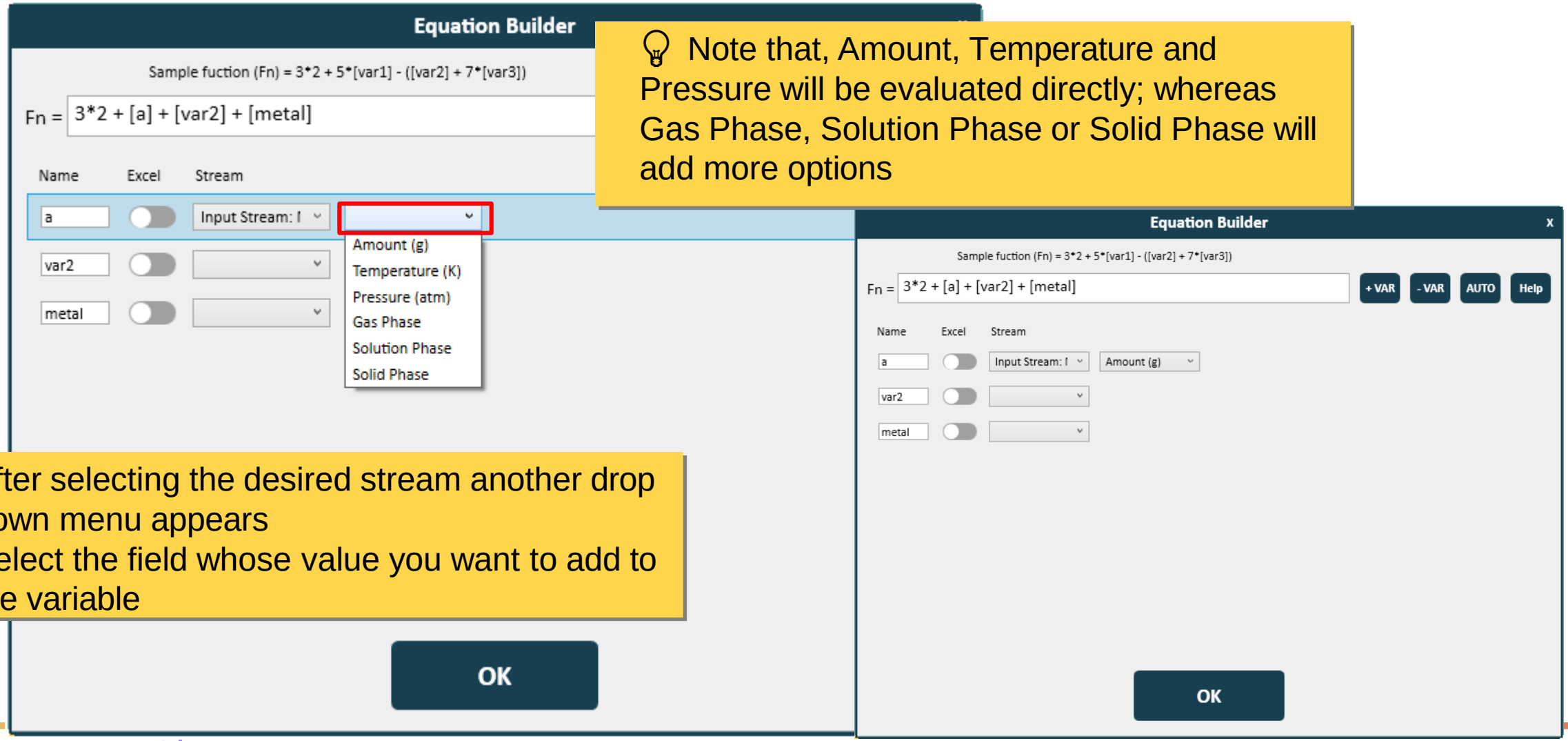
Using Equation: Variable declarations



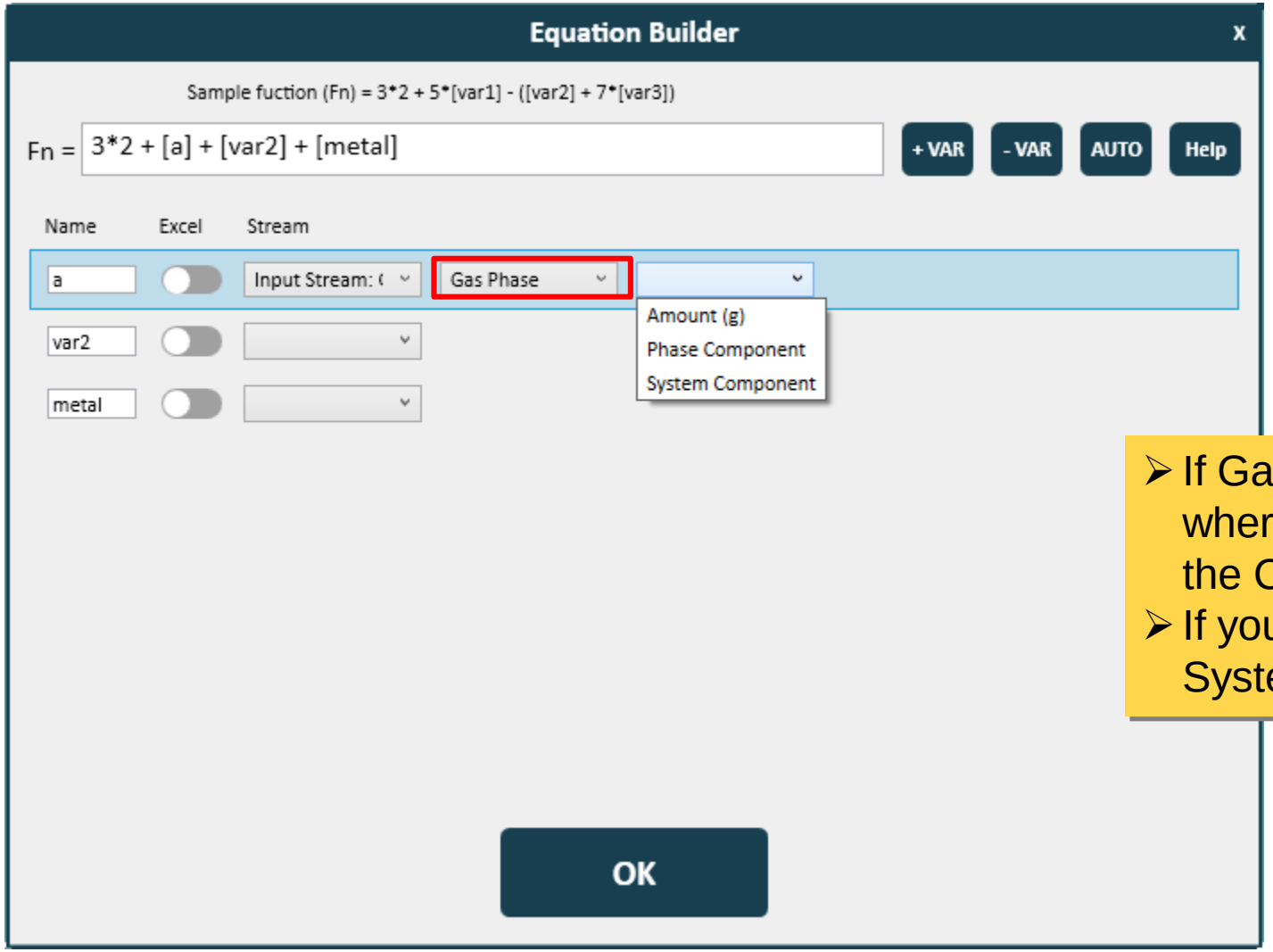
- A list of all the Input Streams and Streams currently part of the process model will pop out after clicking on the drop down menu

  Note that, it shows all streams, regardless of its connection to current module
- Select the desired stream from the list

Using Equation: Variable declarations

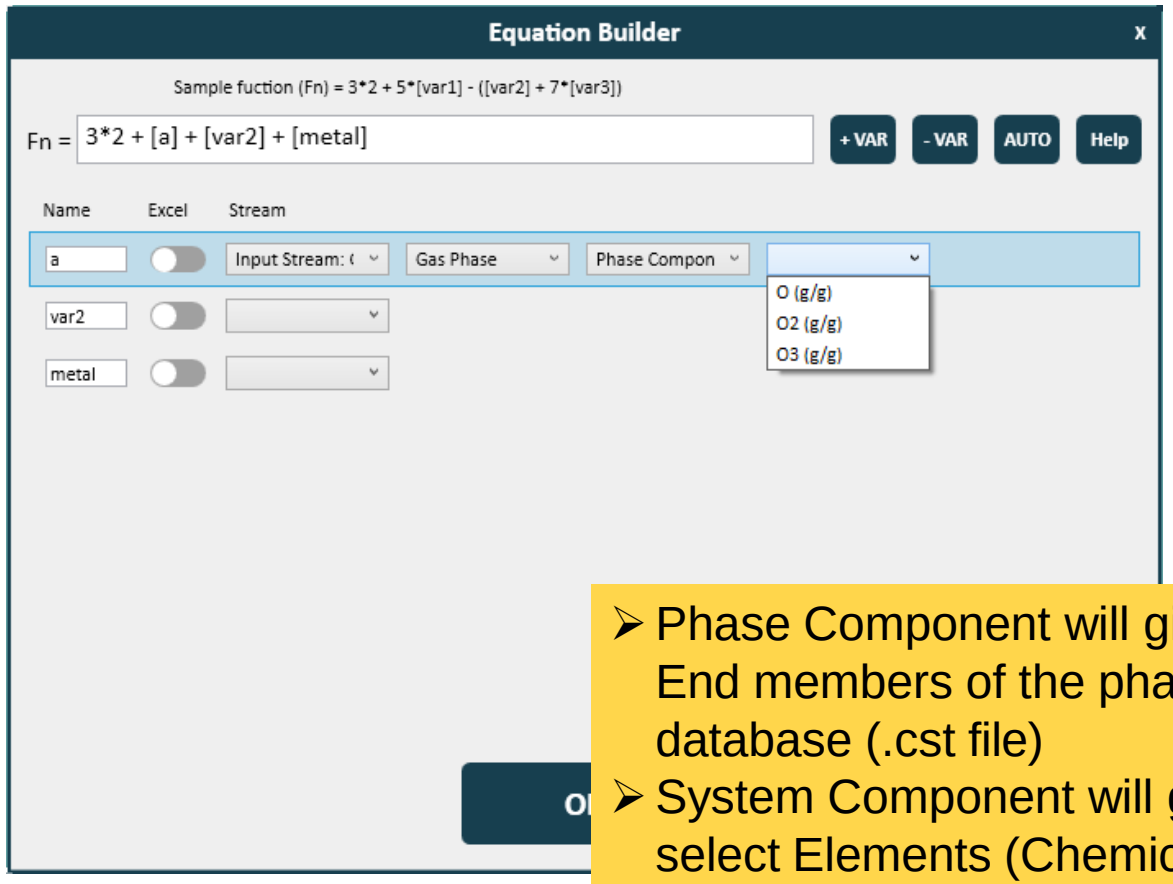


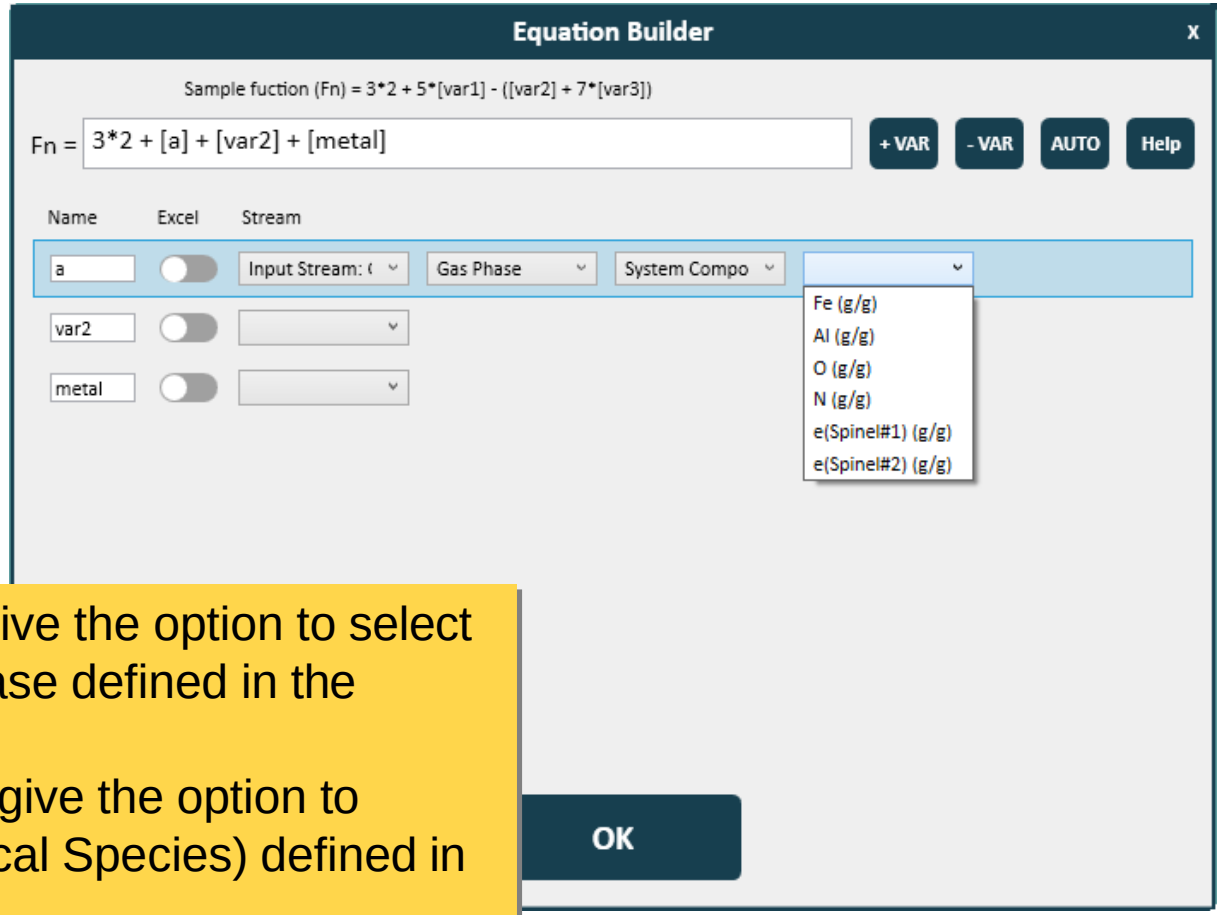
Using Equation: Variable declarations



- 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

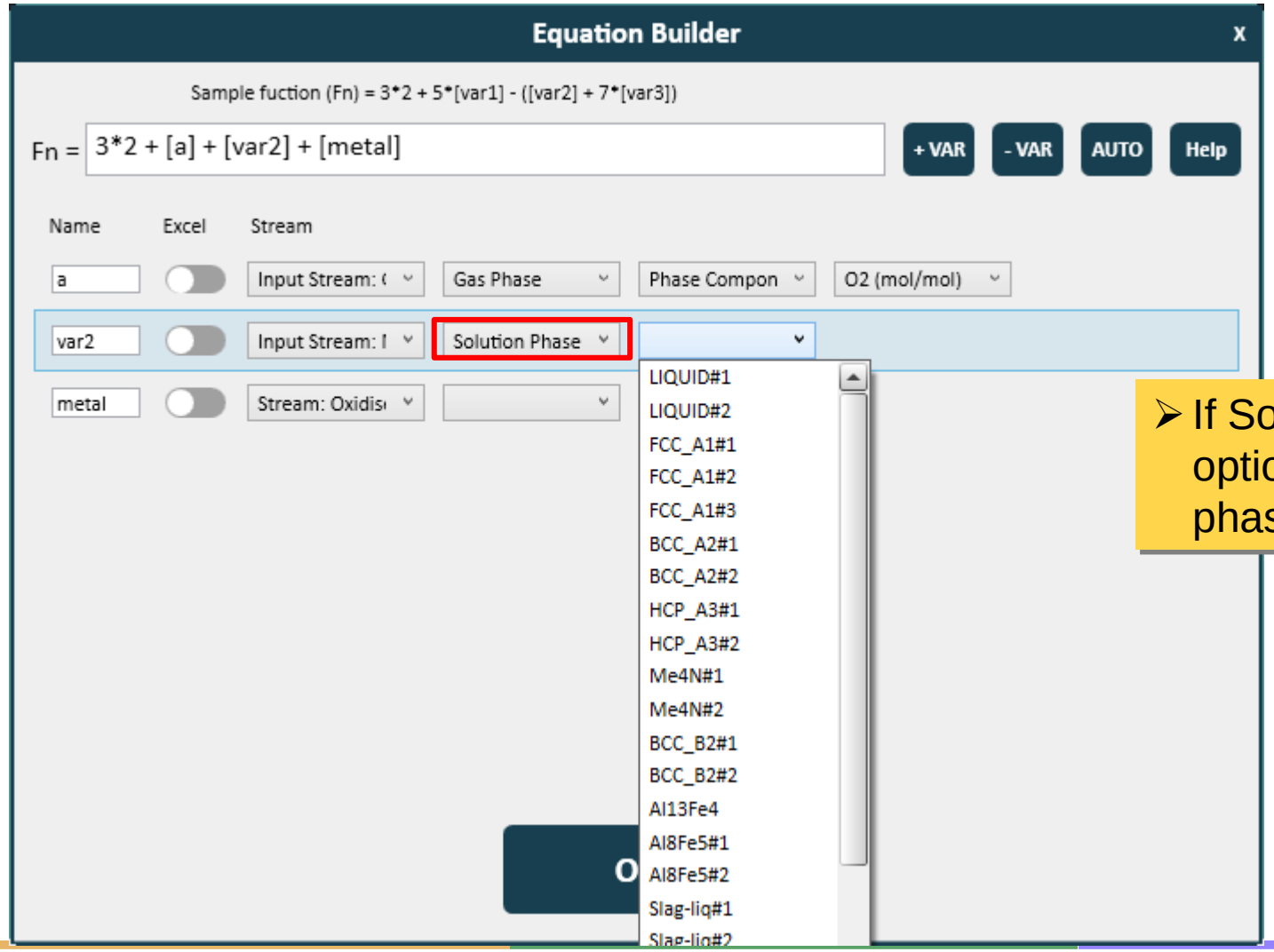
Using Equation: Variable declarations





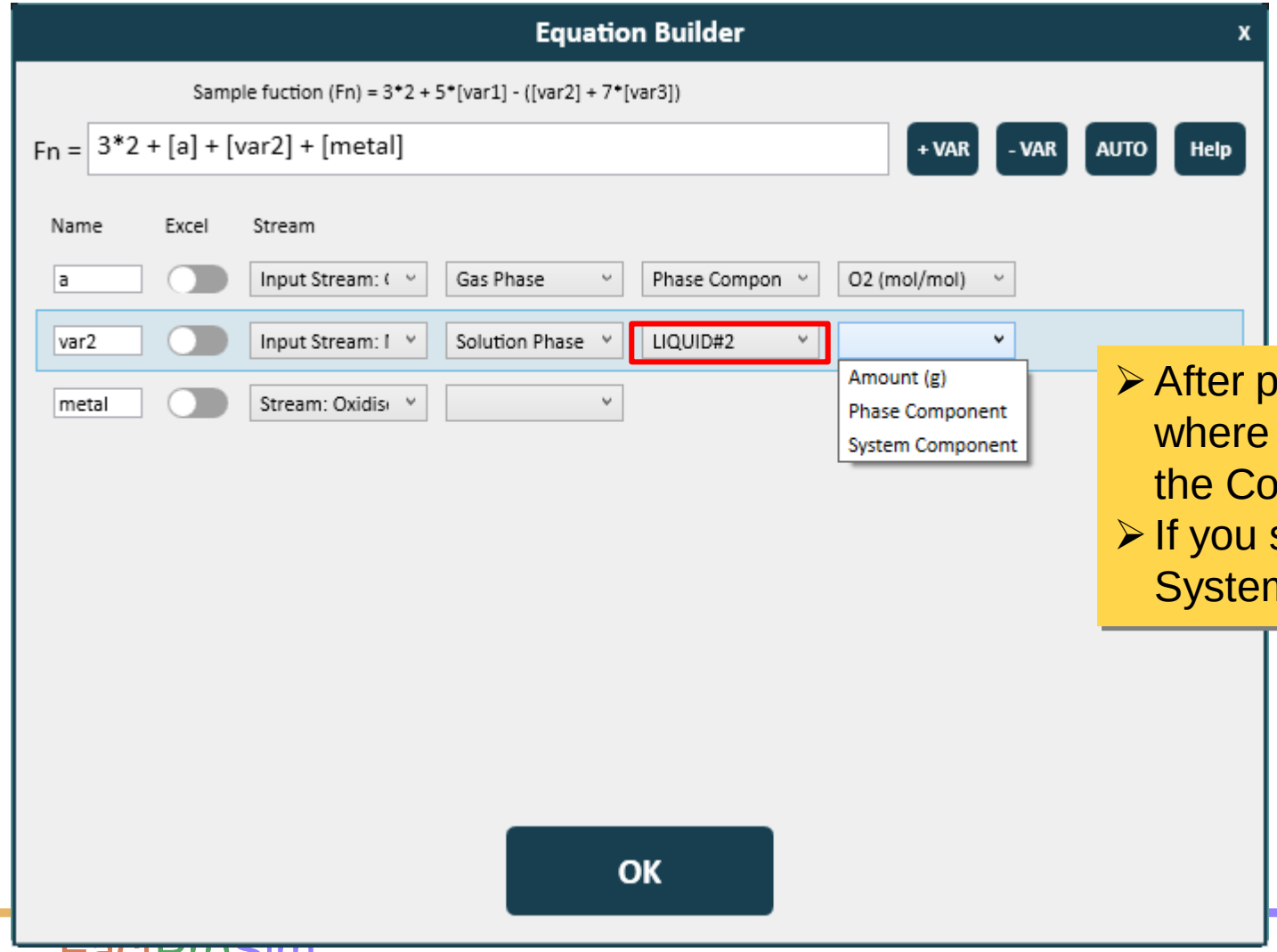
- Phase Component will give the option to select End members of the phase defined in the database (.cst file)
- System Component will give the option to select Elements (Chemical Species) defined in the database (.cst) file

Using Equation: Variable declarations



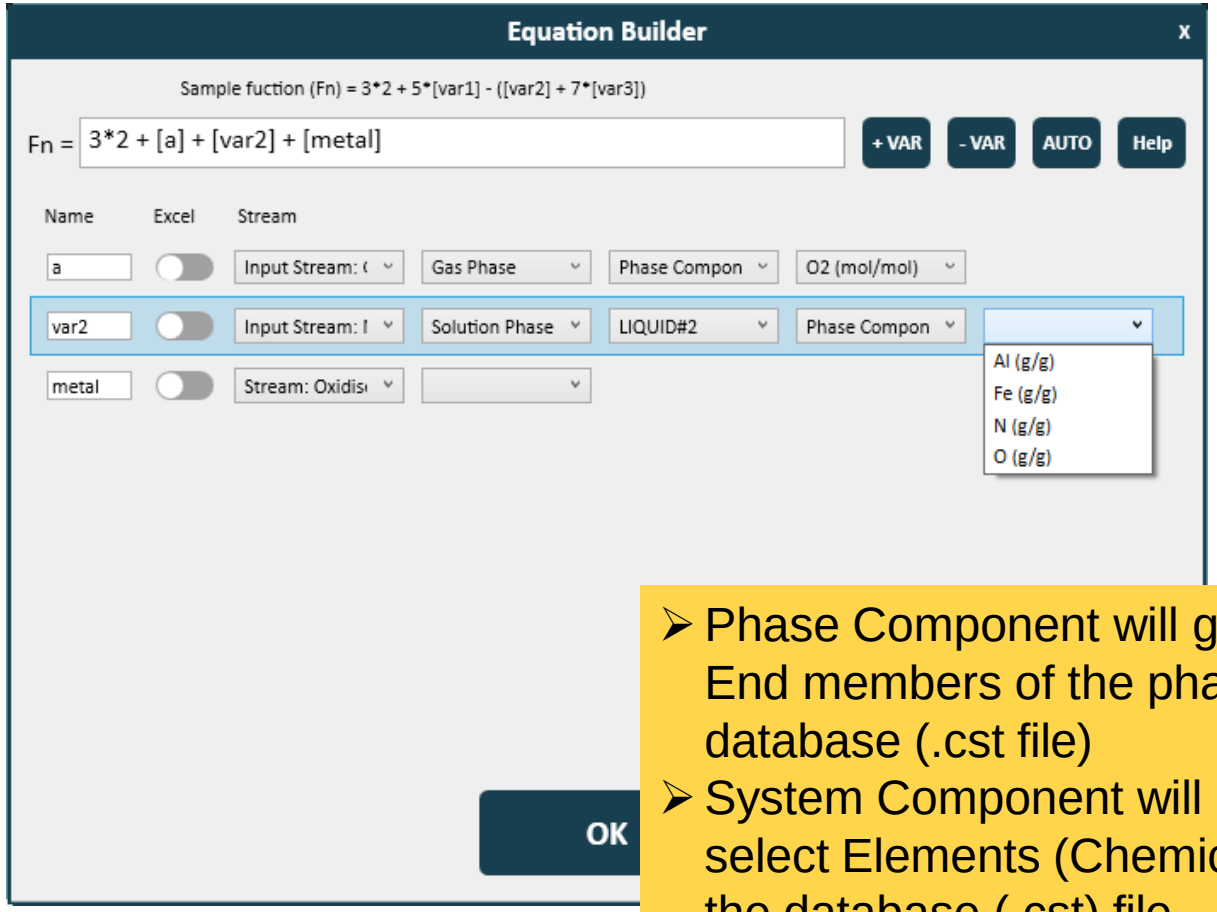
- If Solution Phase is selected it will add extra option, where you can select any solution phase **except** Gas Phase

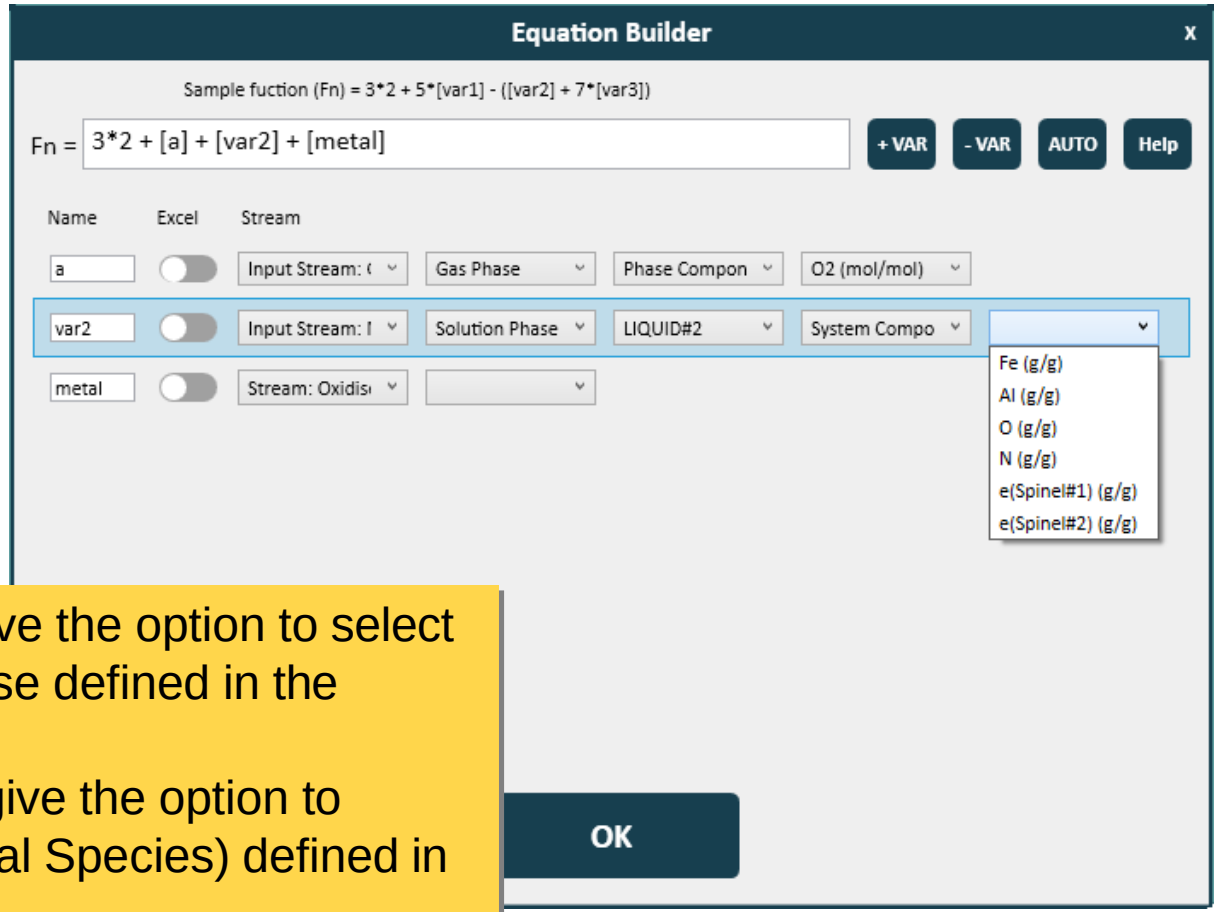
Using Equation: Variable declarations



- 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





- Phase Component will give the option to select End members of the phase defined in the database (.cst file)
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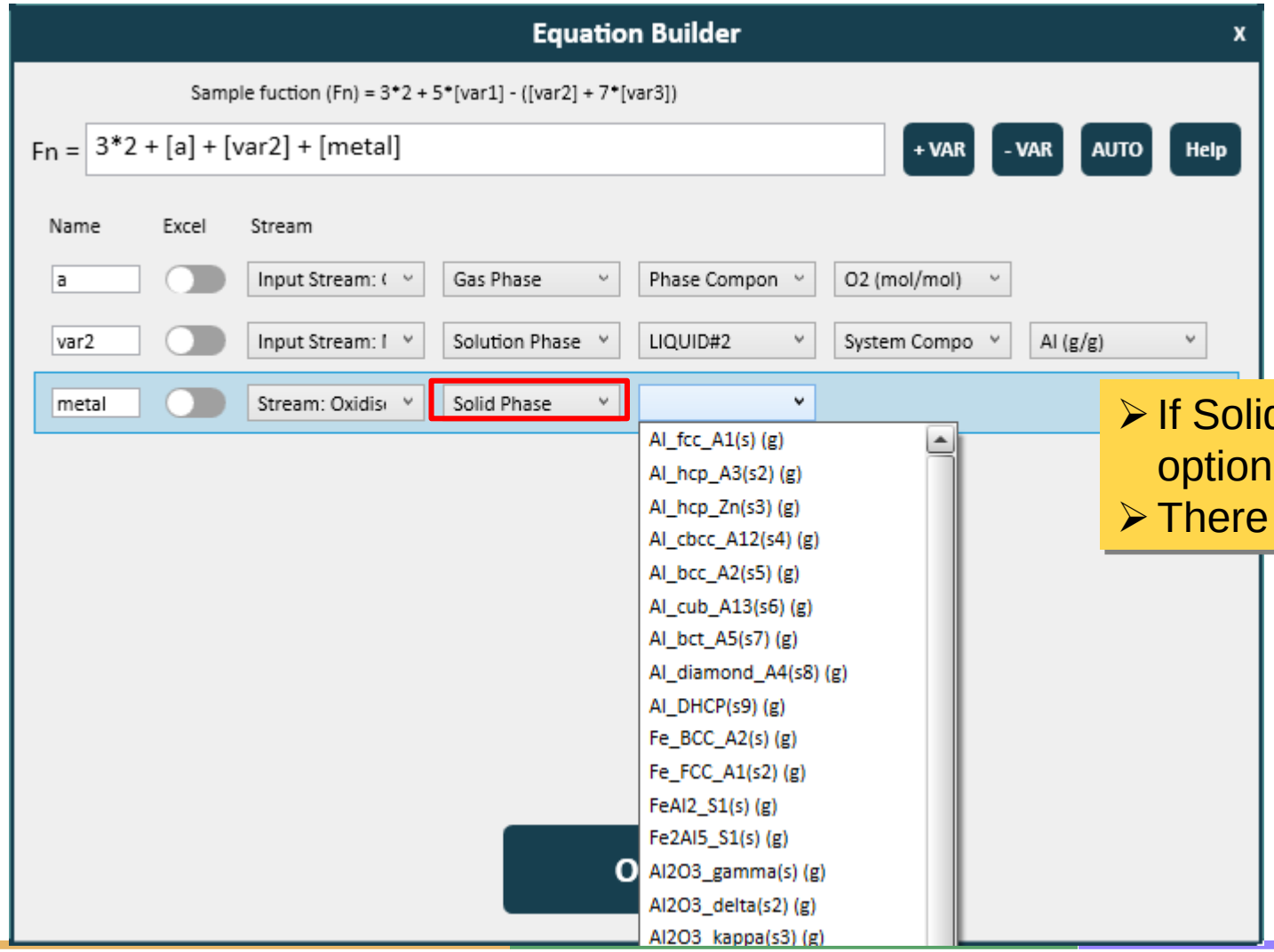
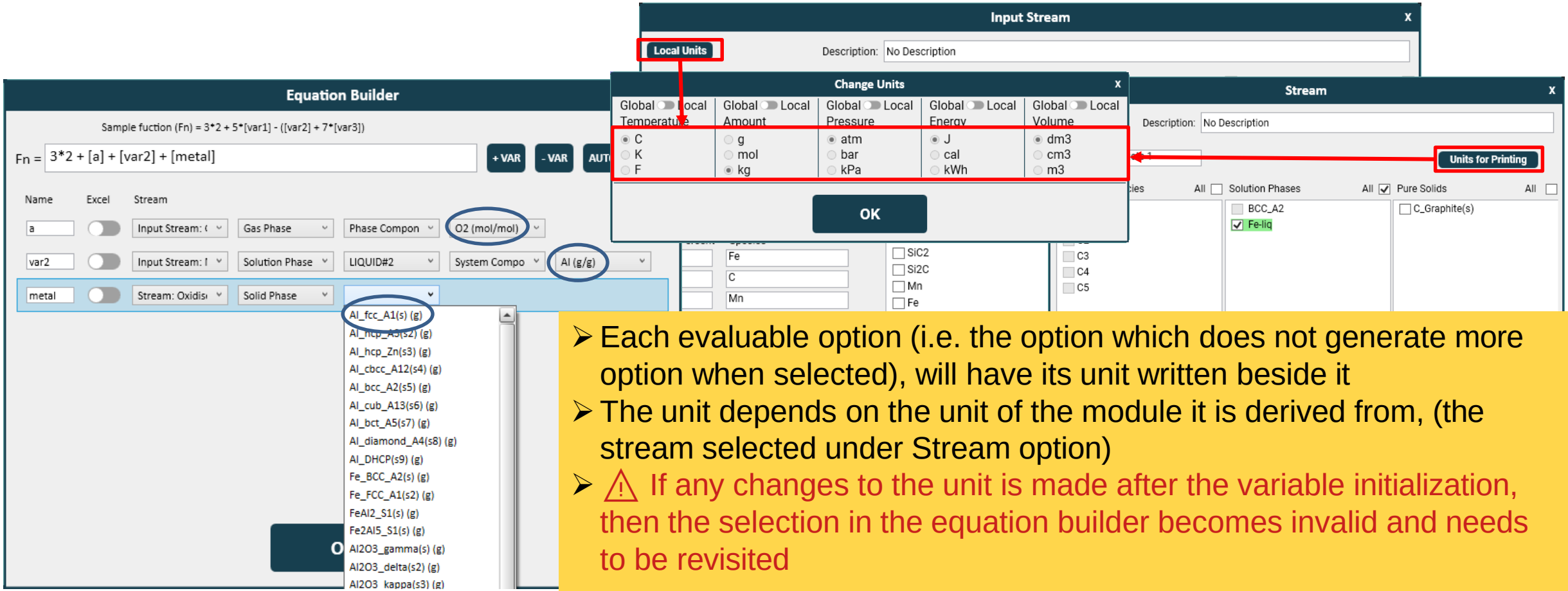
Using Equation: Variable declarations



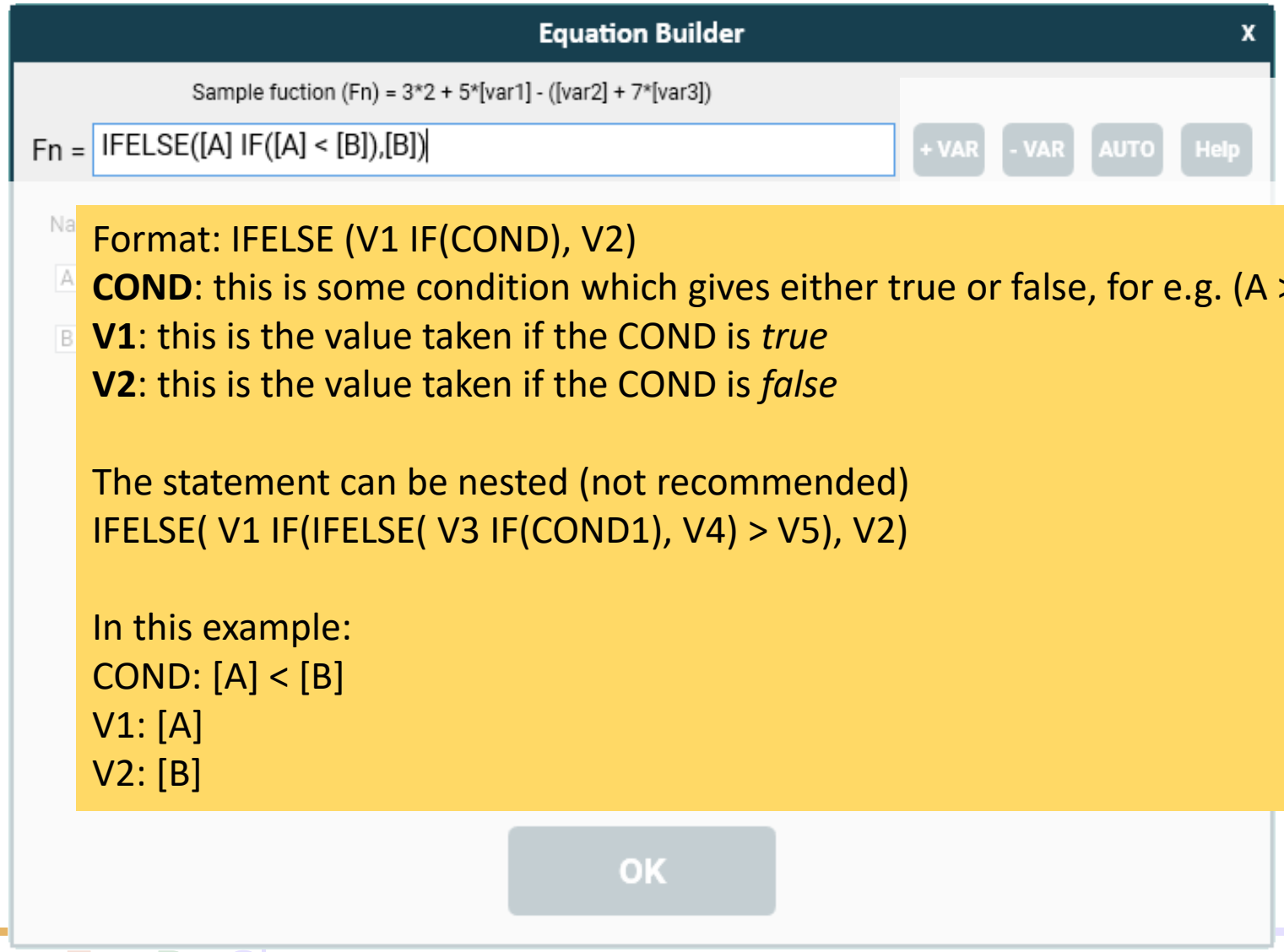
- If Solid Phase is selected it will add extra option, where you can select any solid phase
- There is no other extra option in solid phase

Using Equation: Variable Unit



- 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



Format: IFELSE (V1 IF(COND), V2)
COND: this is some condition which gives either true or false, for e.g. (A > 2)
V1: this is the value taken if the COND is *true*
V2: this is the value taken if the COND is *false*

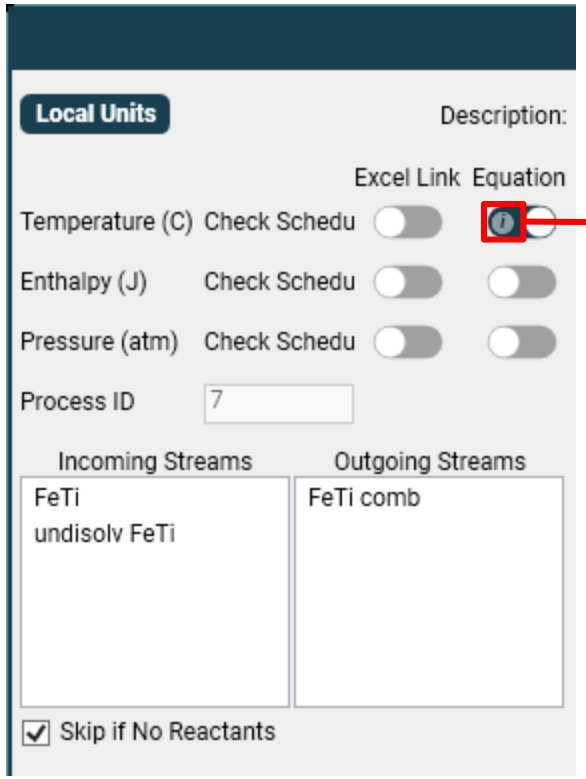
The statement can be nested (not recommended)
IFELSE(V1 IF(IFELSE(V3 IF(COND1), V4) > V5), V2)

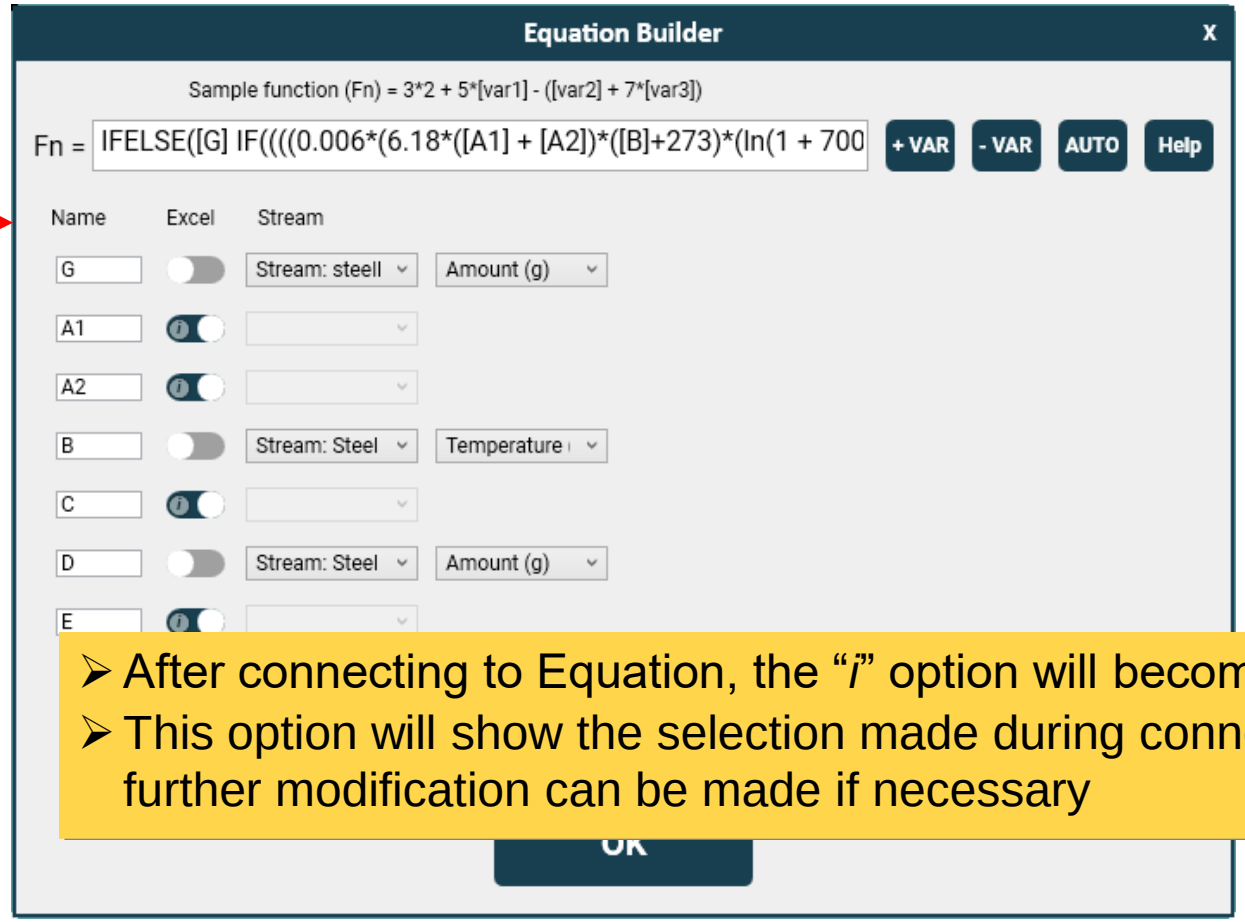
In this example:
COND: [A] < [B]
V1: [A]
V2: [B]

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





- 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

Description of the program

- Overview of the main window and commands in the Toolbar
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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
  - Align the process modules in the flowsheet
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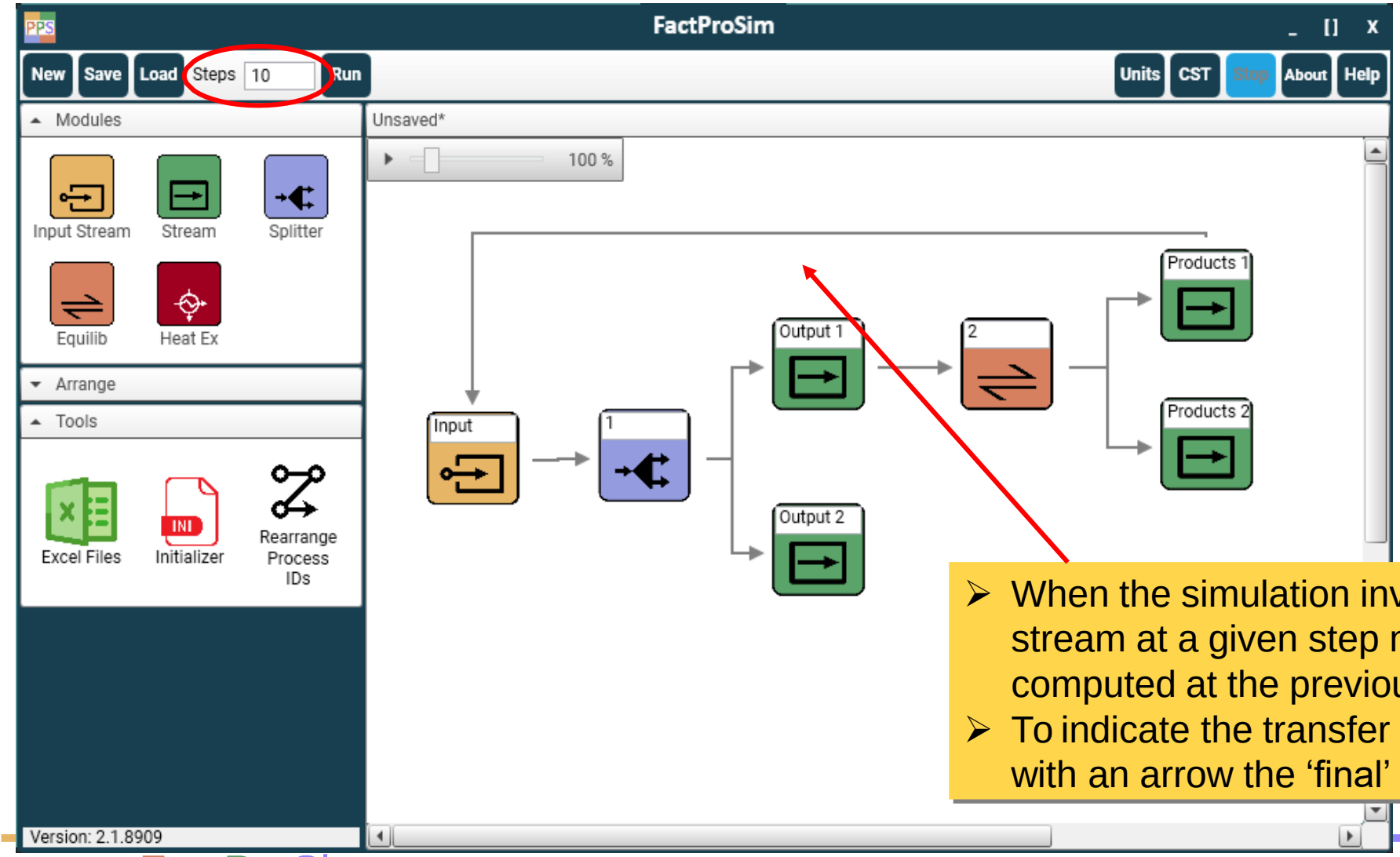
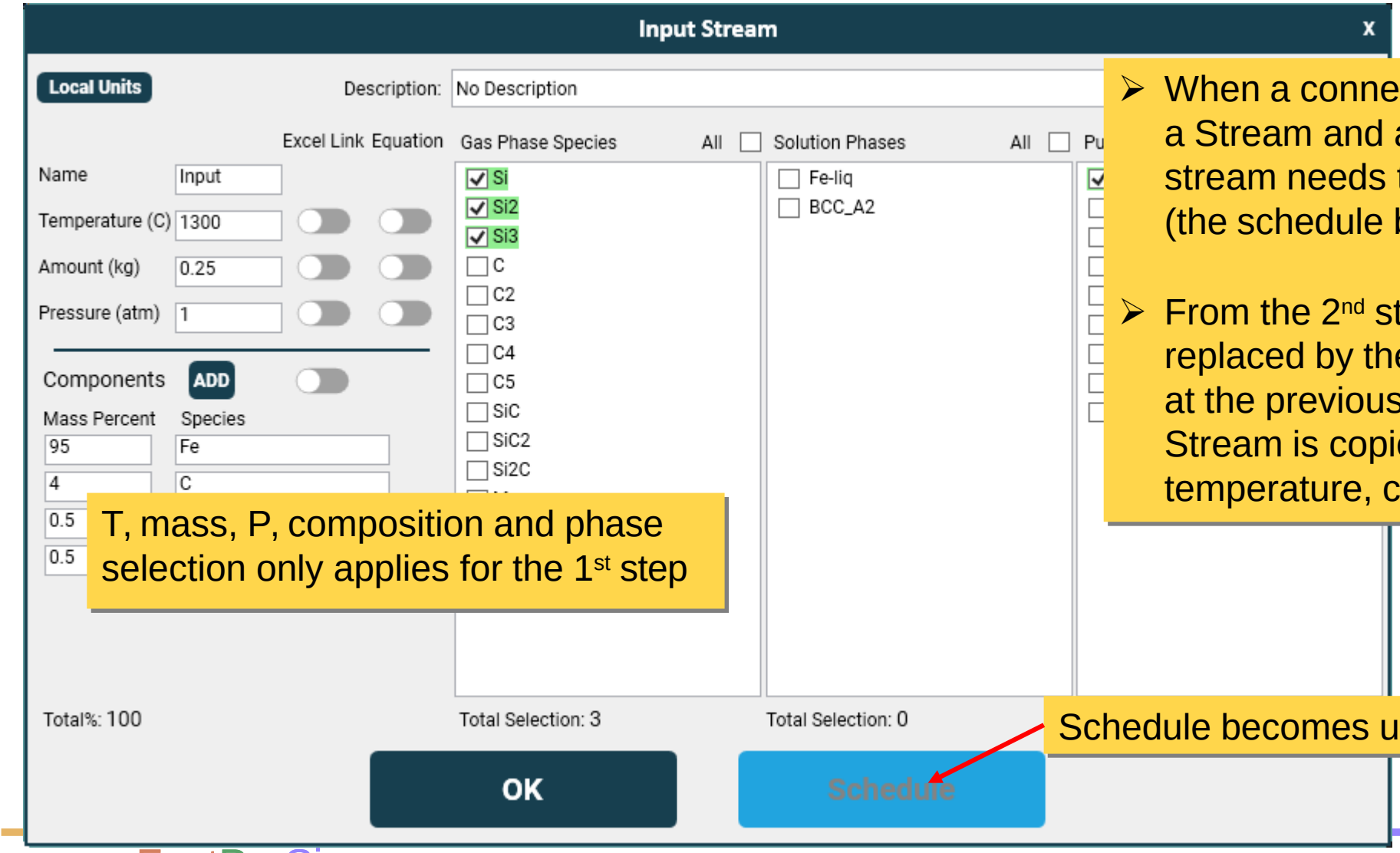
Transferring material to the next step



- When the simulation involves multiple time steps, an input stream at a given step might by 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



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

- 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

Schedule becomes unavailable

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  - **Changing global and local units**
  - Manage Splitter and Equilib Process IDs
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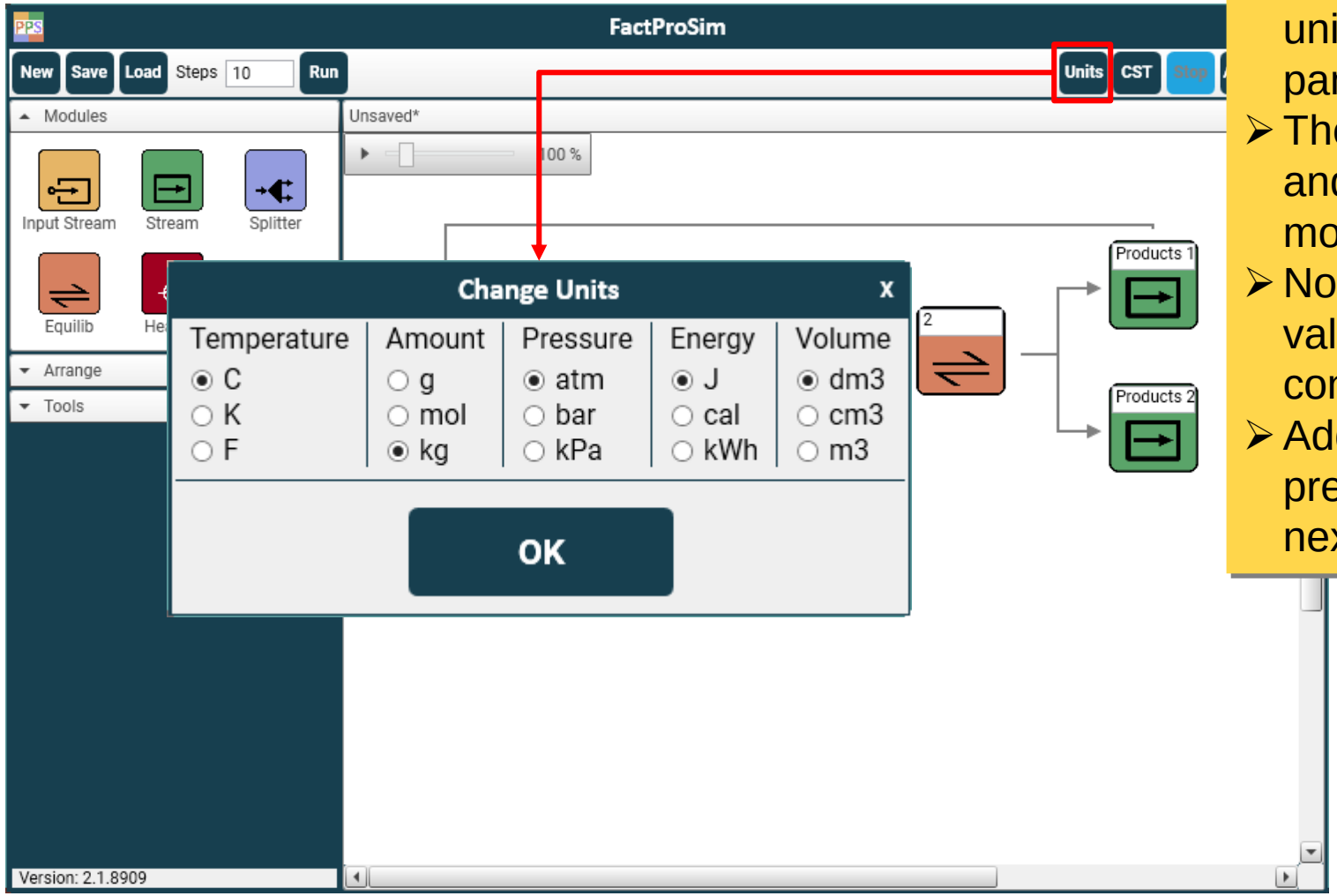
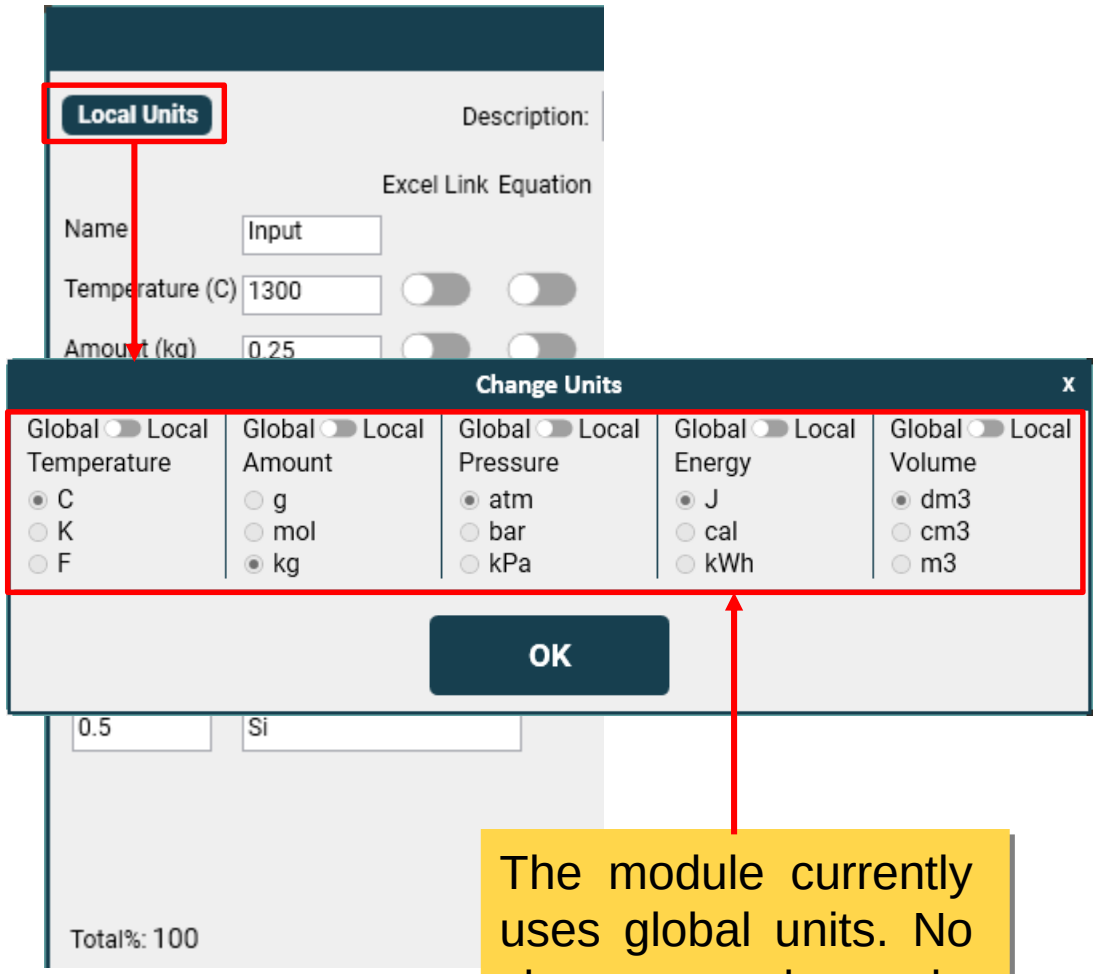
Global Units



- 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



The module currently uses global units. No changes can be made

- 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

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  - **Manage Splitter and Equilib Process IDs**
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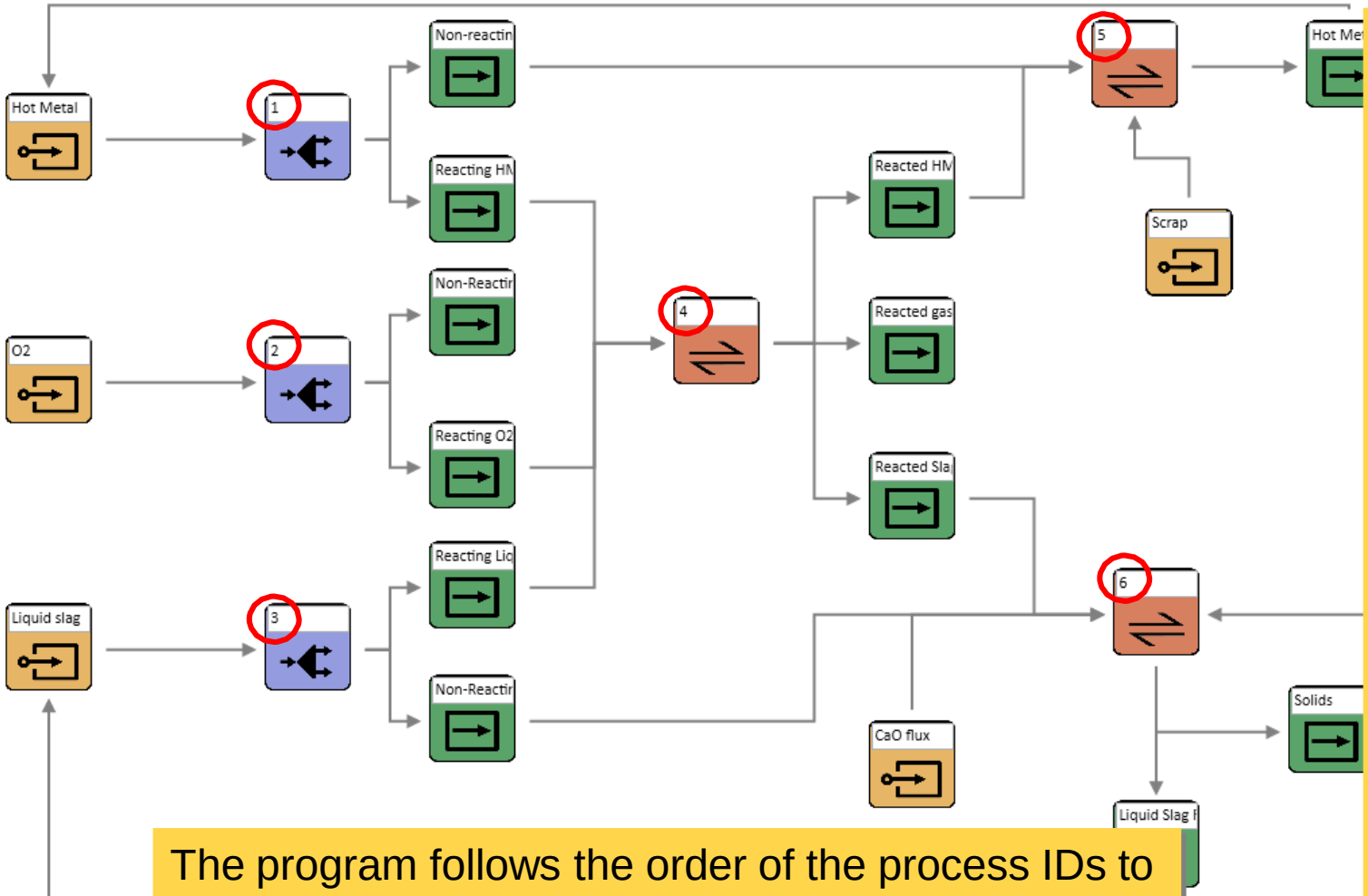
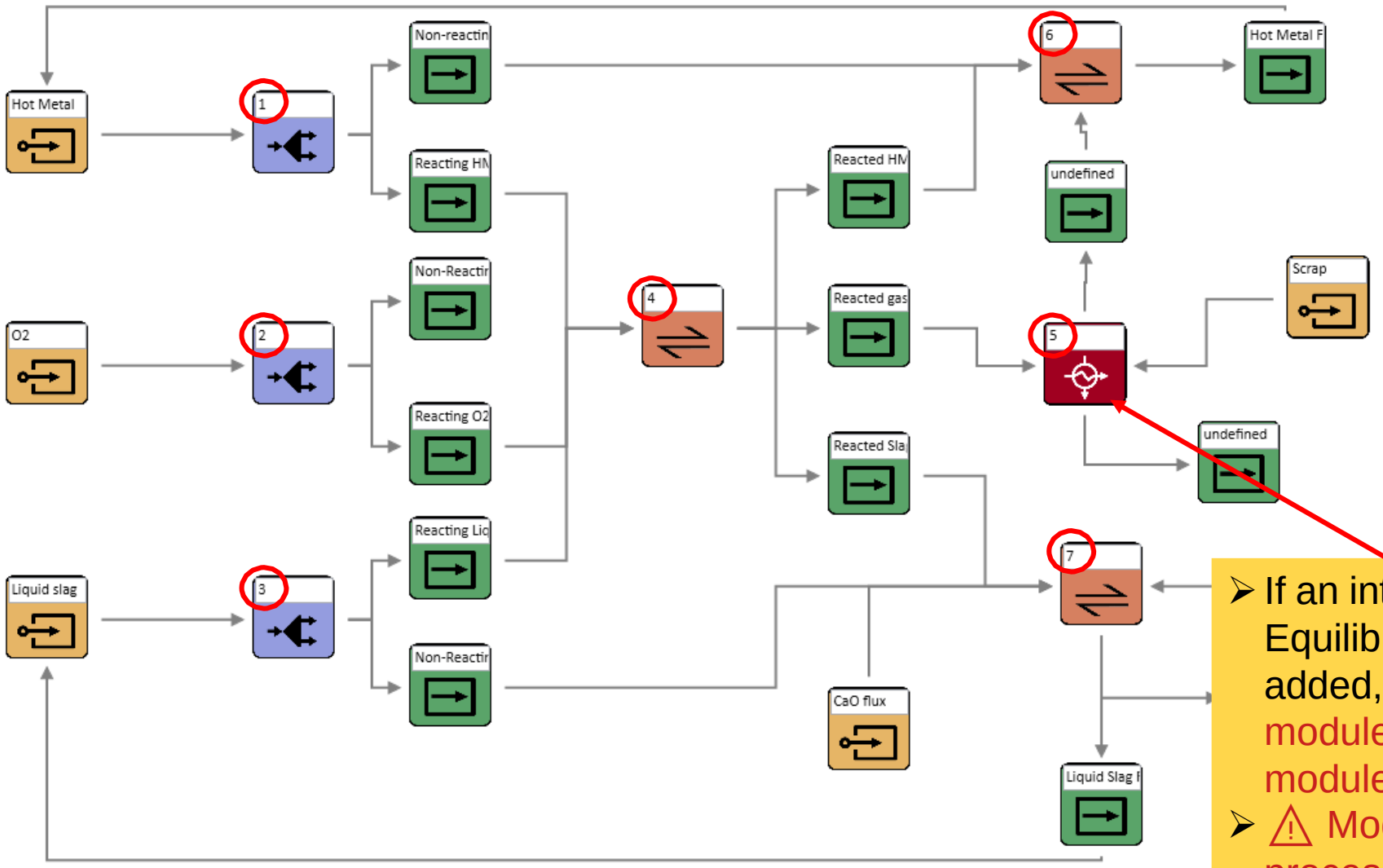
Splitter and Equilib process IDs



The program follows the order of the process IDs to perform the operations designed in the flowsheet

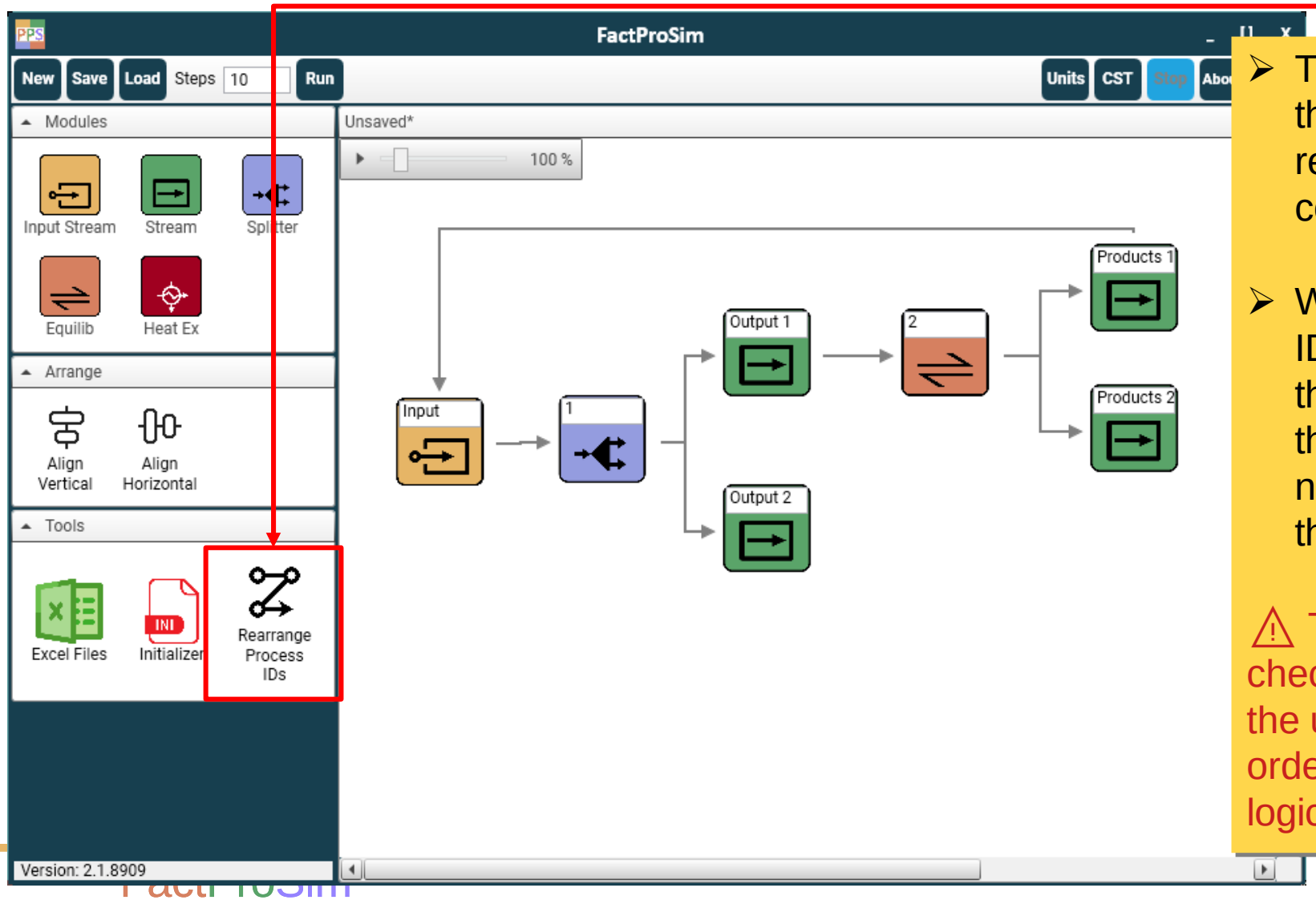
- To perform the calculations designed in the process flowsheet, the program must execute the operations according to the order set in the flowsheet
- However, at this moment, the program cannot navigate the flowsheet and figure on its own in which order the operations must performed
- The splitter and Equilib modules have a unique process ID which tells the program in which order they should be calculated
- The process ID is attributed to each splitter and Equilib when inserted in the Diagram workspace
- ⚠ It is the user's responsibility to check that the process IDs are in order

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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  - Changing global and local units
  - Manage Splitter and Equilib Process IDs
  - **Align the process modules in the flowsheet**
  - Save and load an existing flowsheet
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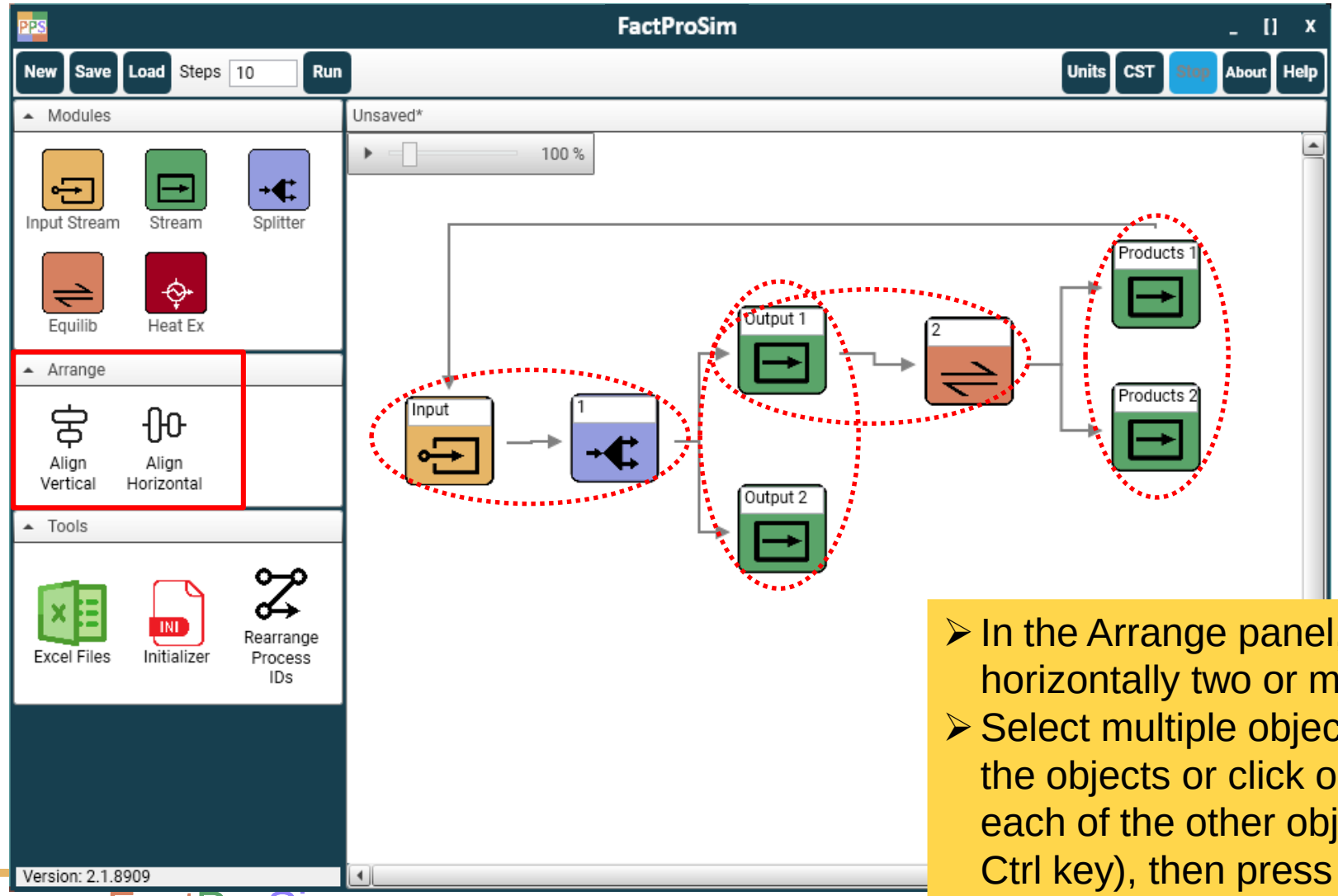
Align the modules in the diagram



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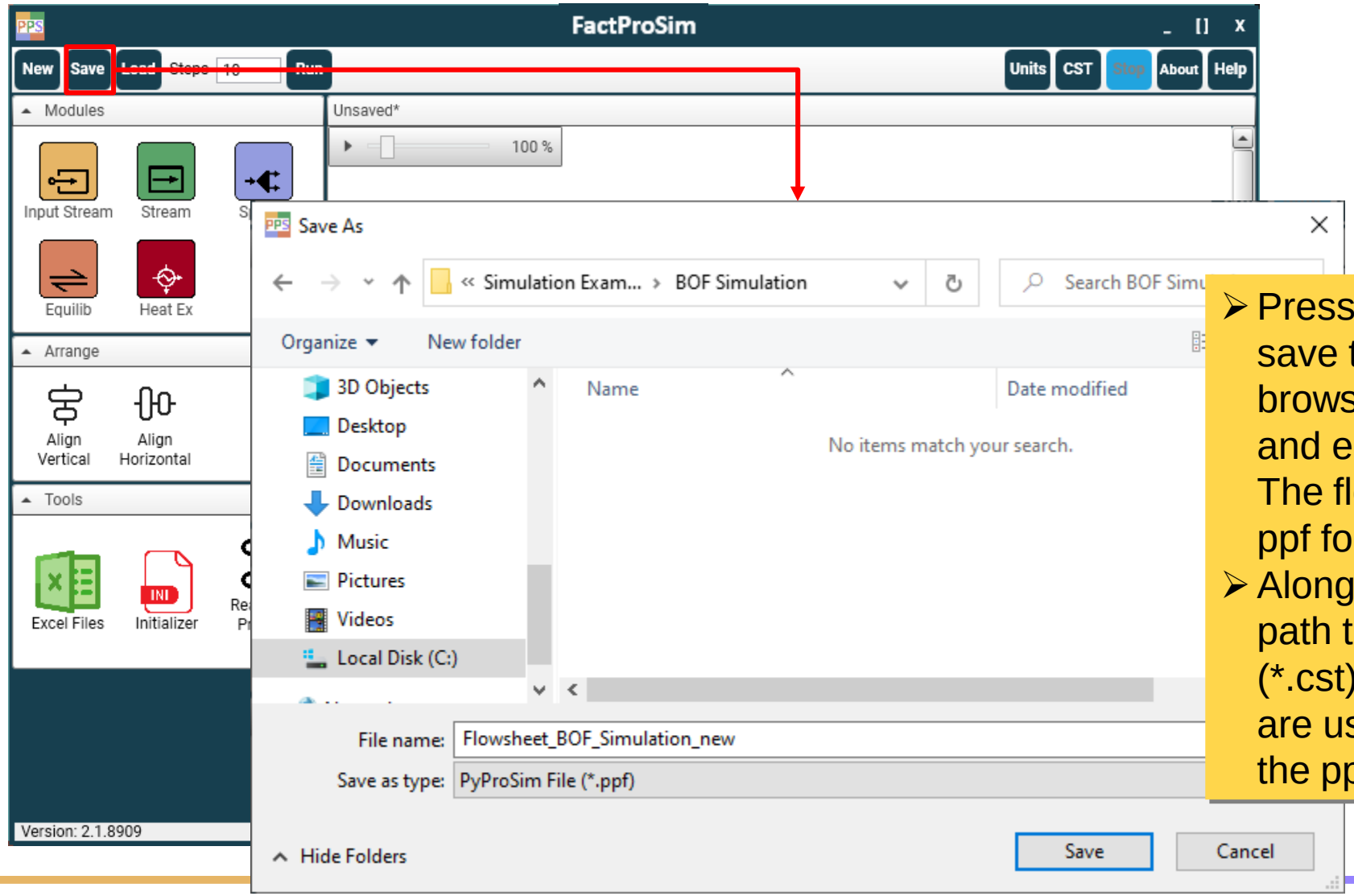
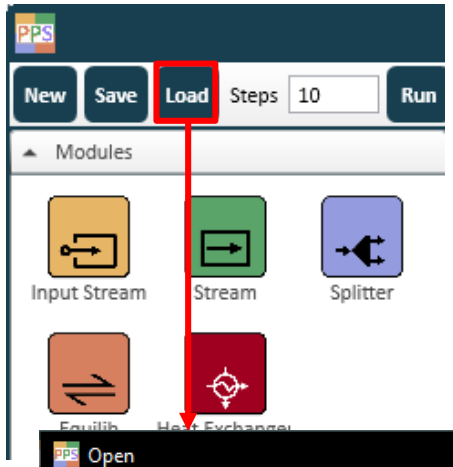
- Step 5: View the Results (Output Excel File)

Save the flowsheet

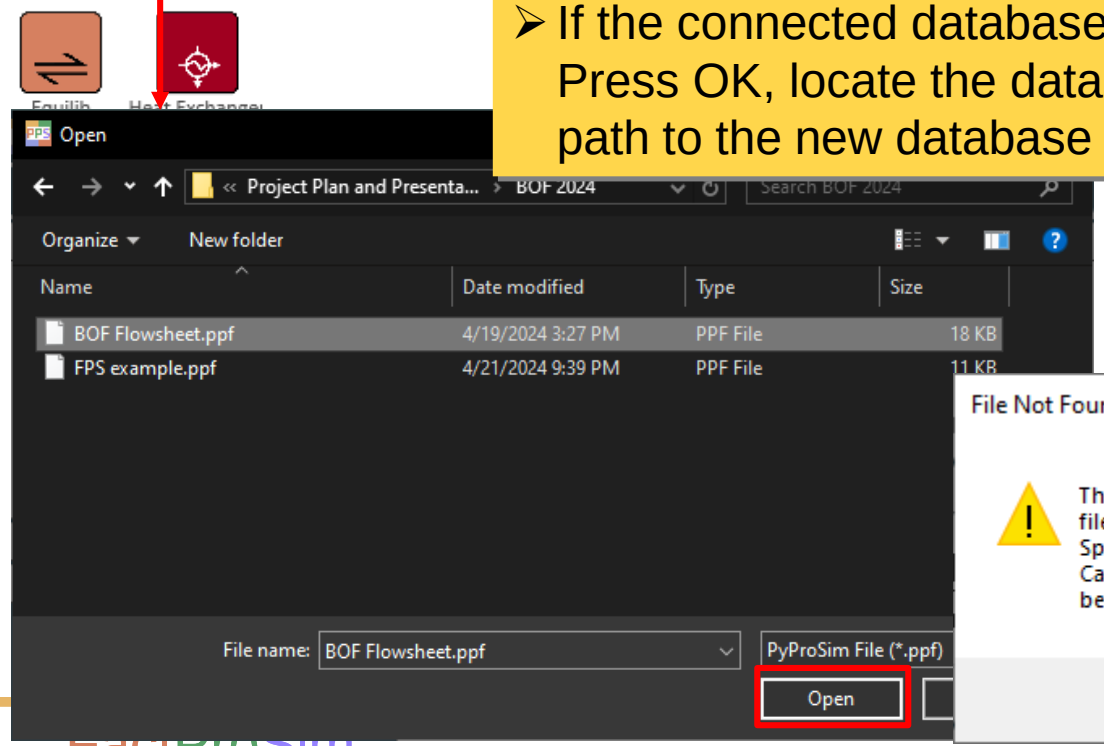


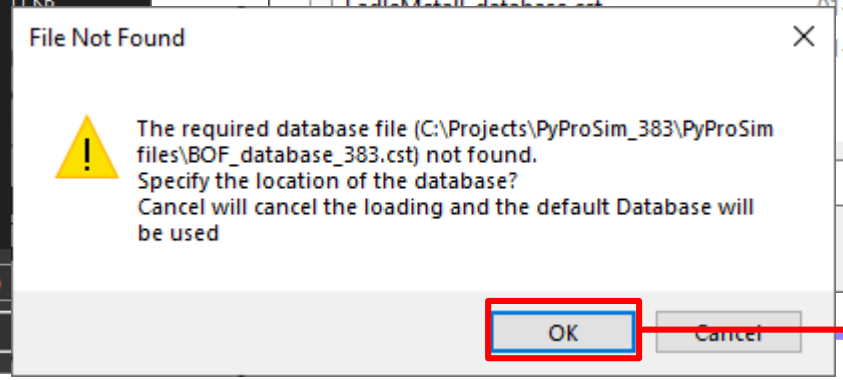
- Press the button Save in the toolbar to save the current flowsheet. In the browse window, select the location and enter the name of the flowsheet. The flowsheet information are saved in ppf format (encrypted)
- Along with all the modules data, the path to the selected database file (*.cst) and Excel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

Load an existing flowsheet



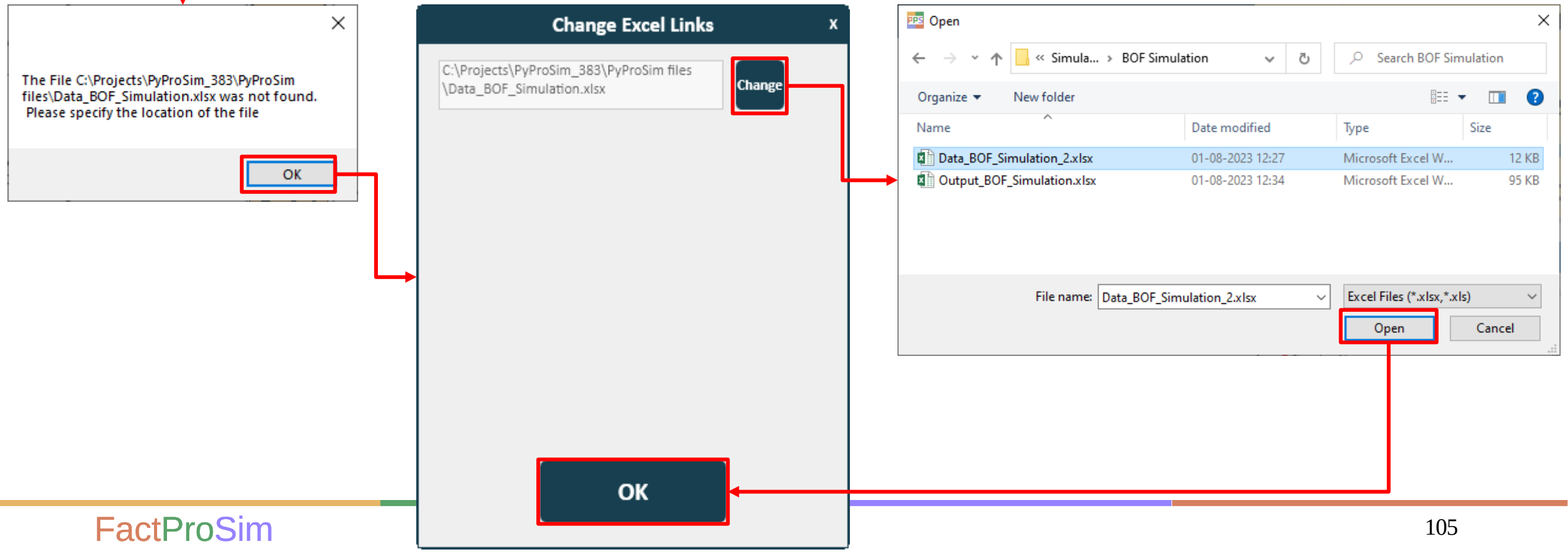
- Press the button Load in the toolbar to open an existing flowsheet. In the browse window, select the flowsheet to open (in ppf format) ⚠ The current flowsheet will be lost if not saved!
- Each flowsheet is connected to a database file (*.cst) and Excel Files (if Excel Links are used in the modules). 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)

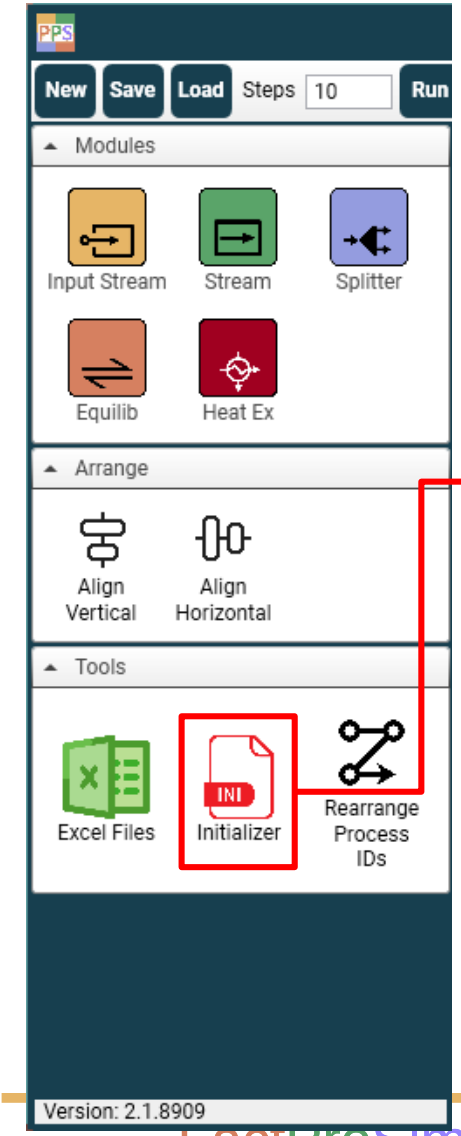
- Similarly, if the connected Excel file(s) is not found, the program will prompt to locate the File(s). After pressing OK, the Excel File tool will open automatically. Press the button Change next to the Excel File path. In the browse window, locate the Excel file and press Open. The path to the new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

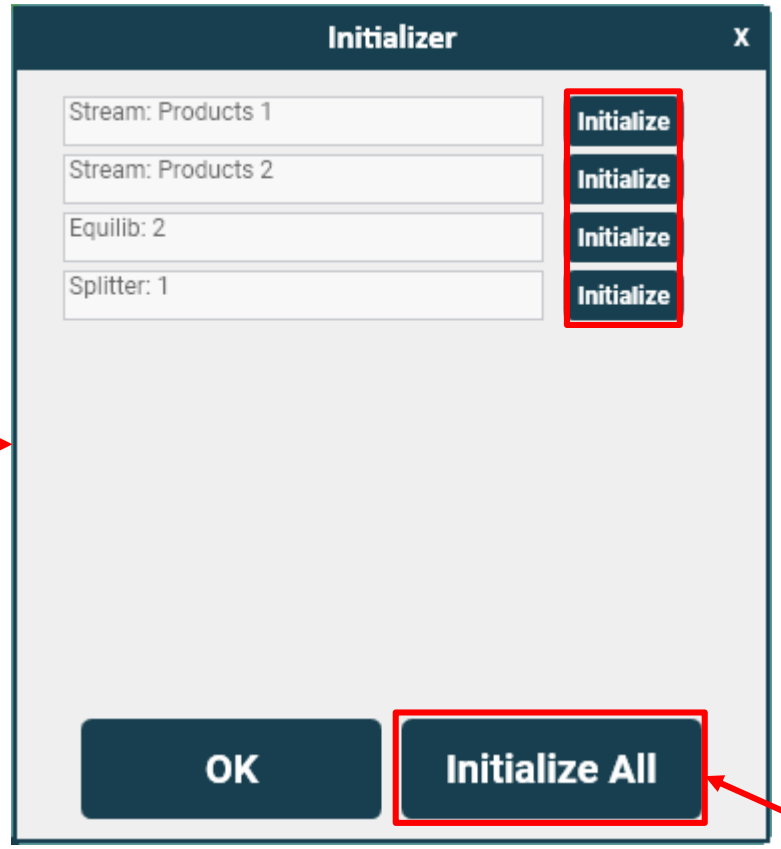


Description of the program

- 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)

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

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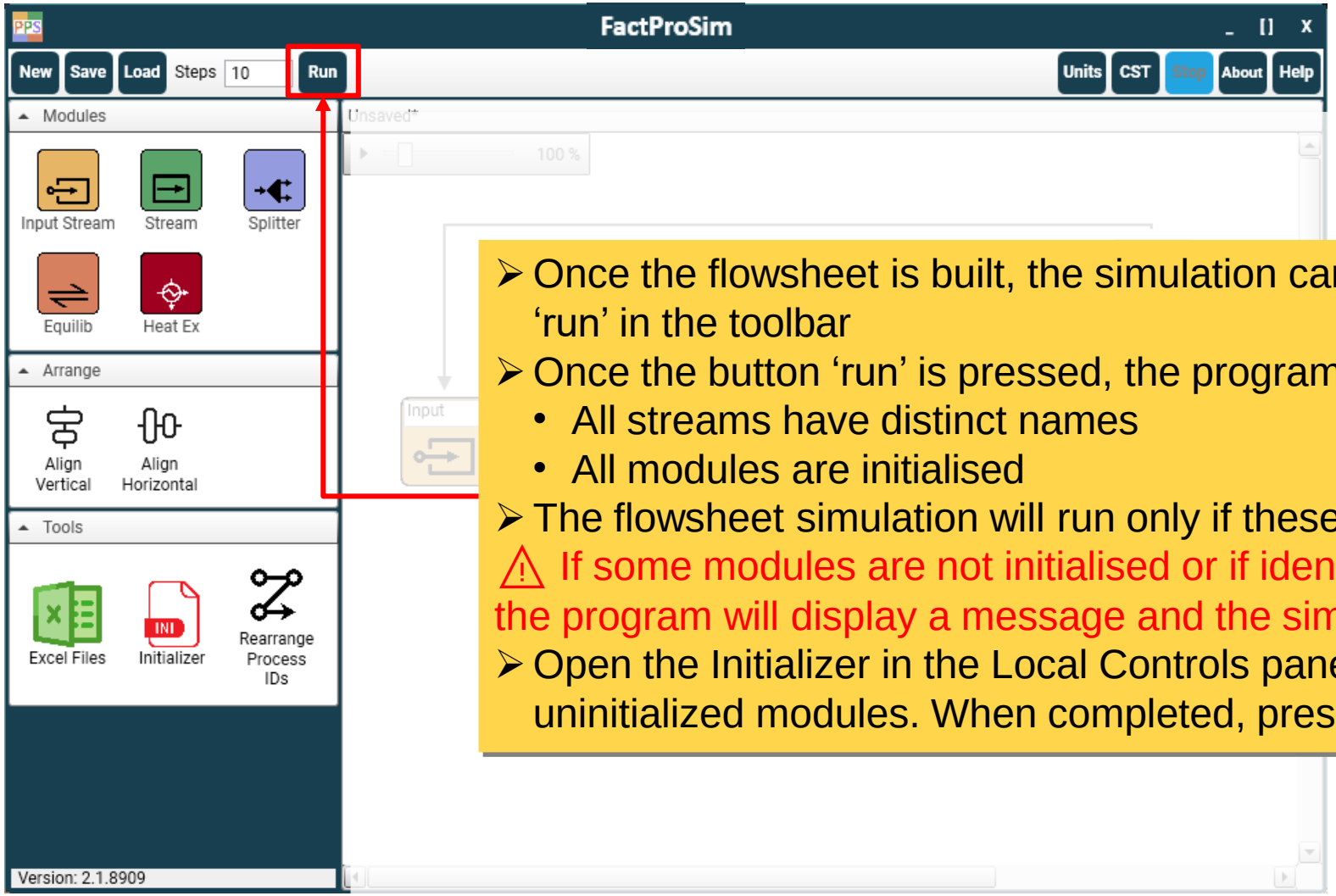
- **Step 4: Run the process flowsheet**
- Step 5: View the Results (Output Excel File)

Step 4: Run the process flowsheet

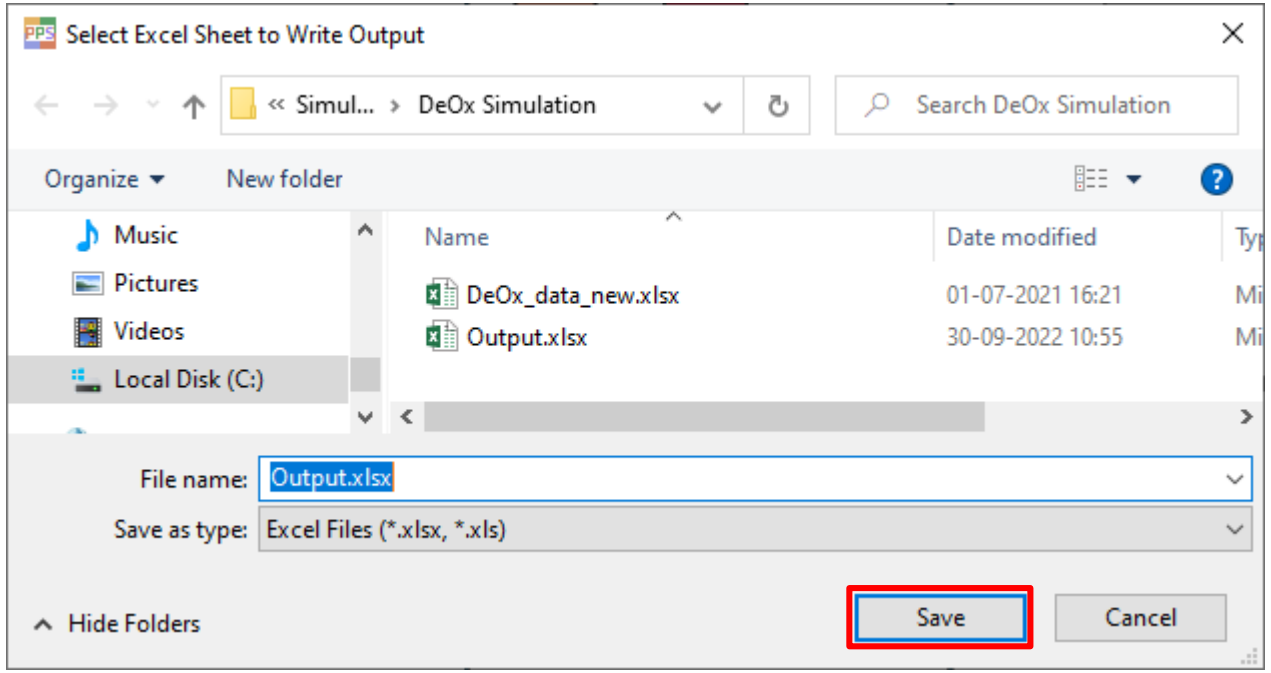


- Once the flowsheet is built, the simulation can be started by clicking the button 'run' in the toolbar
- Once the button 'run' is pressed, the program first do several checks:
  - All streams have distinct names
  - All modules are initialised
- The flowsheet simulation will run only if these checks 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

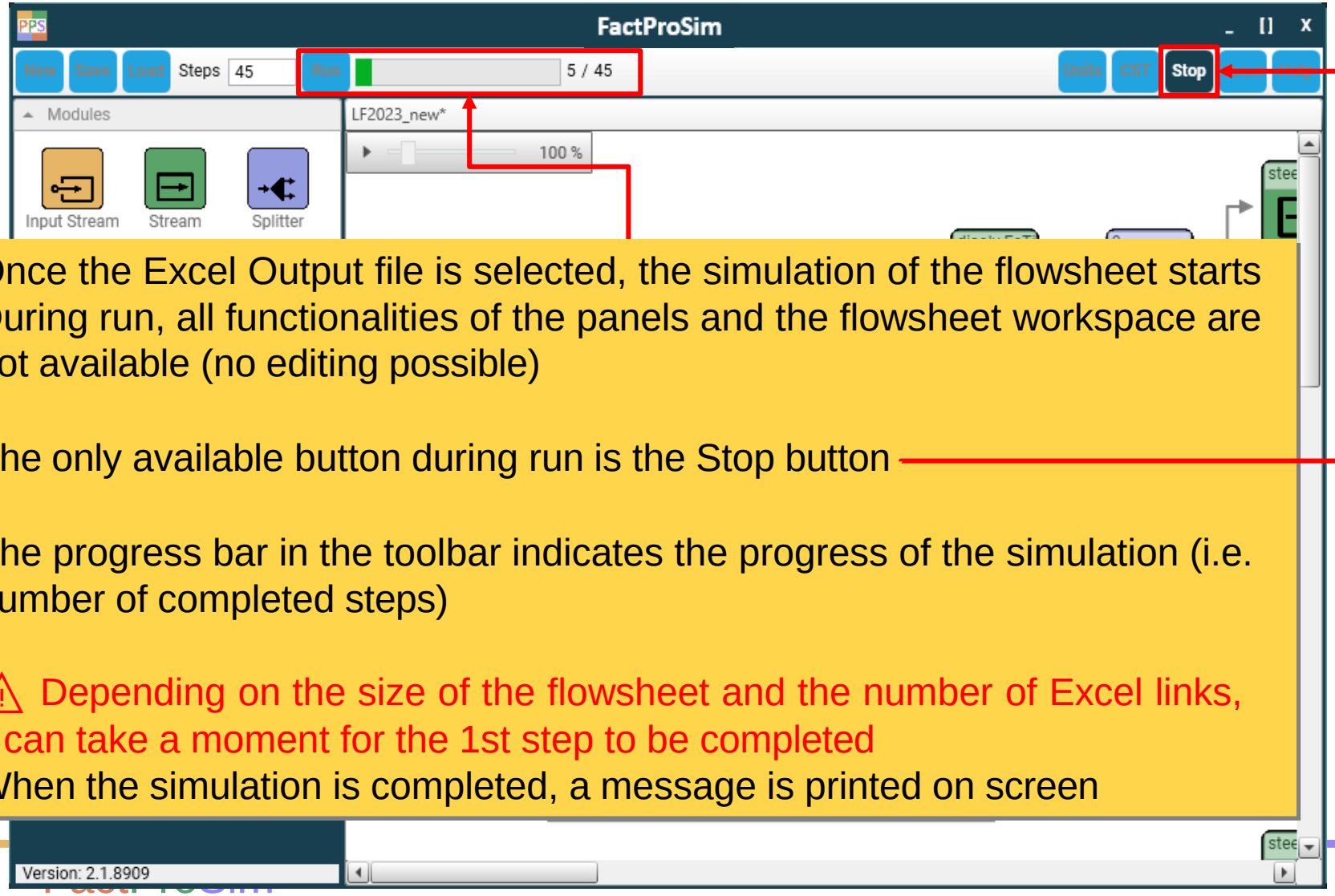
Run the process flowsheet



- 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

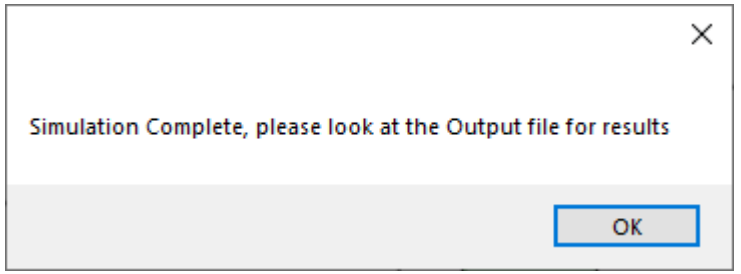


Once the Excel Output file is selected, the simulation of the flowsheet starts
During run, all functionalities of the panels and the flowsheet workspace are not available (no editing possible)

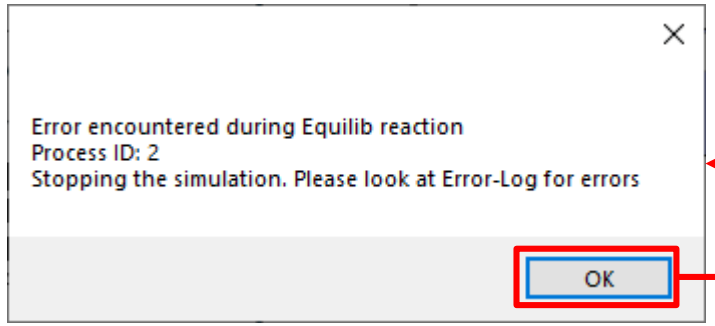
The only available button during run is the Stop button

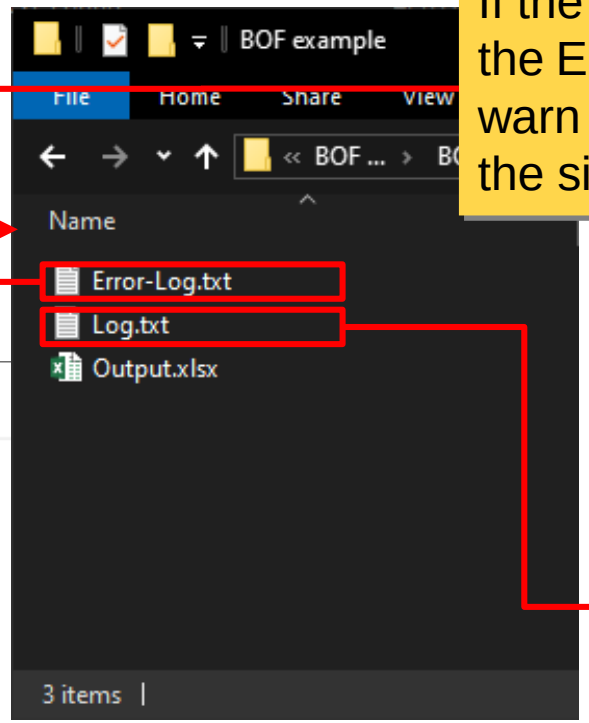
The progress bar in the toolbar indicates the progress of the simulation (i.e. number of completed steps)

⚠ 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

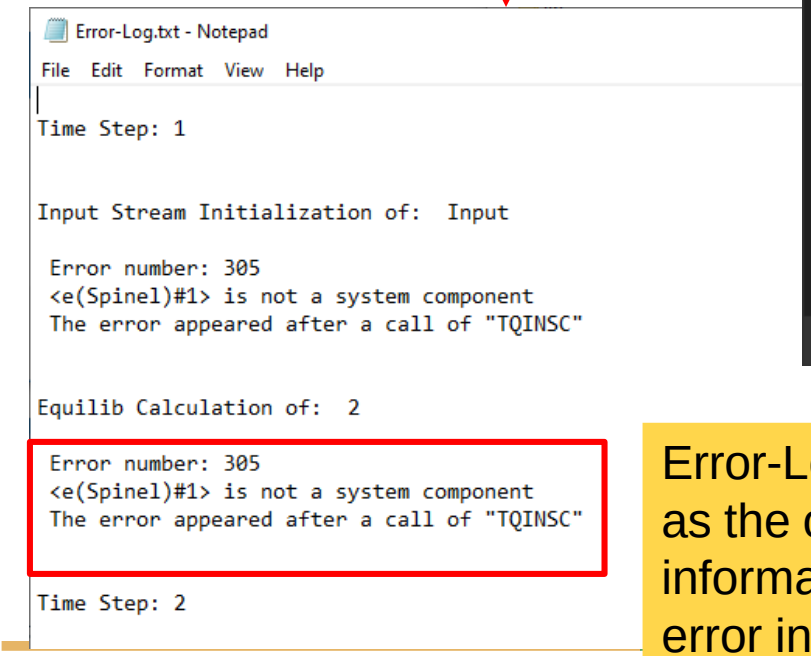


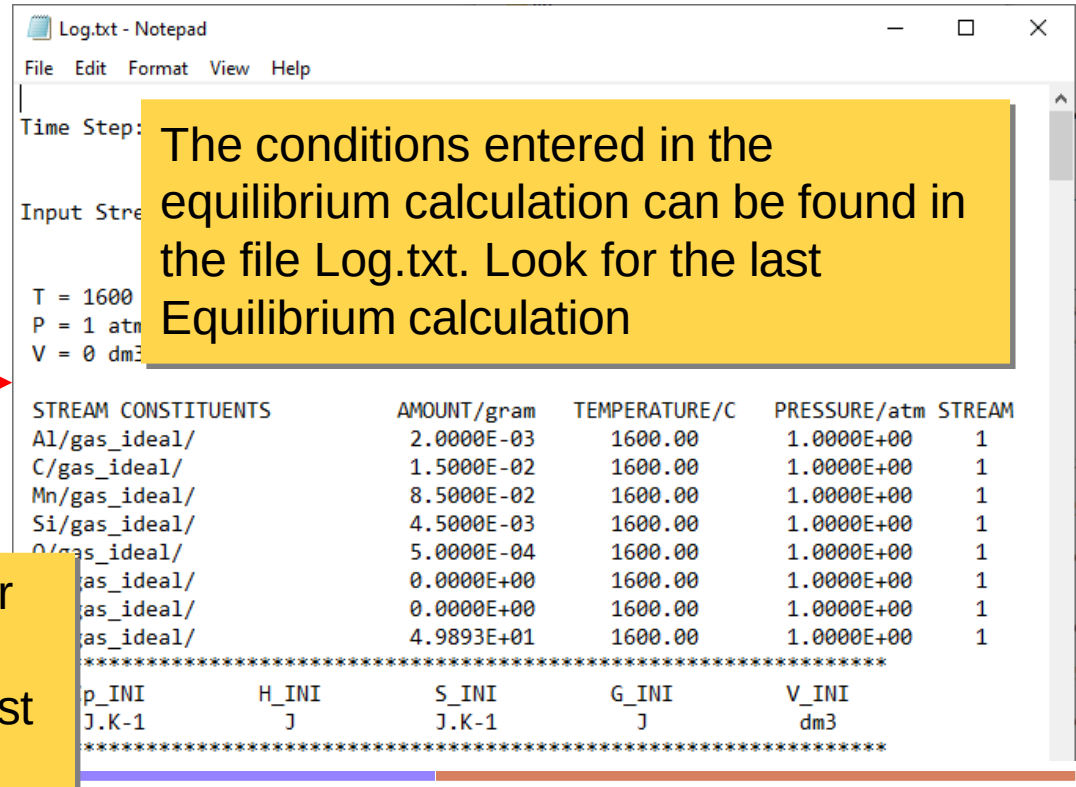
Error during run





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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  - Changing global and local units
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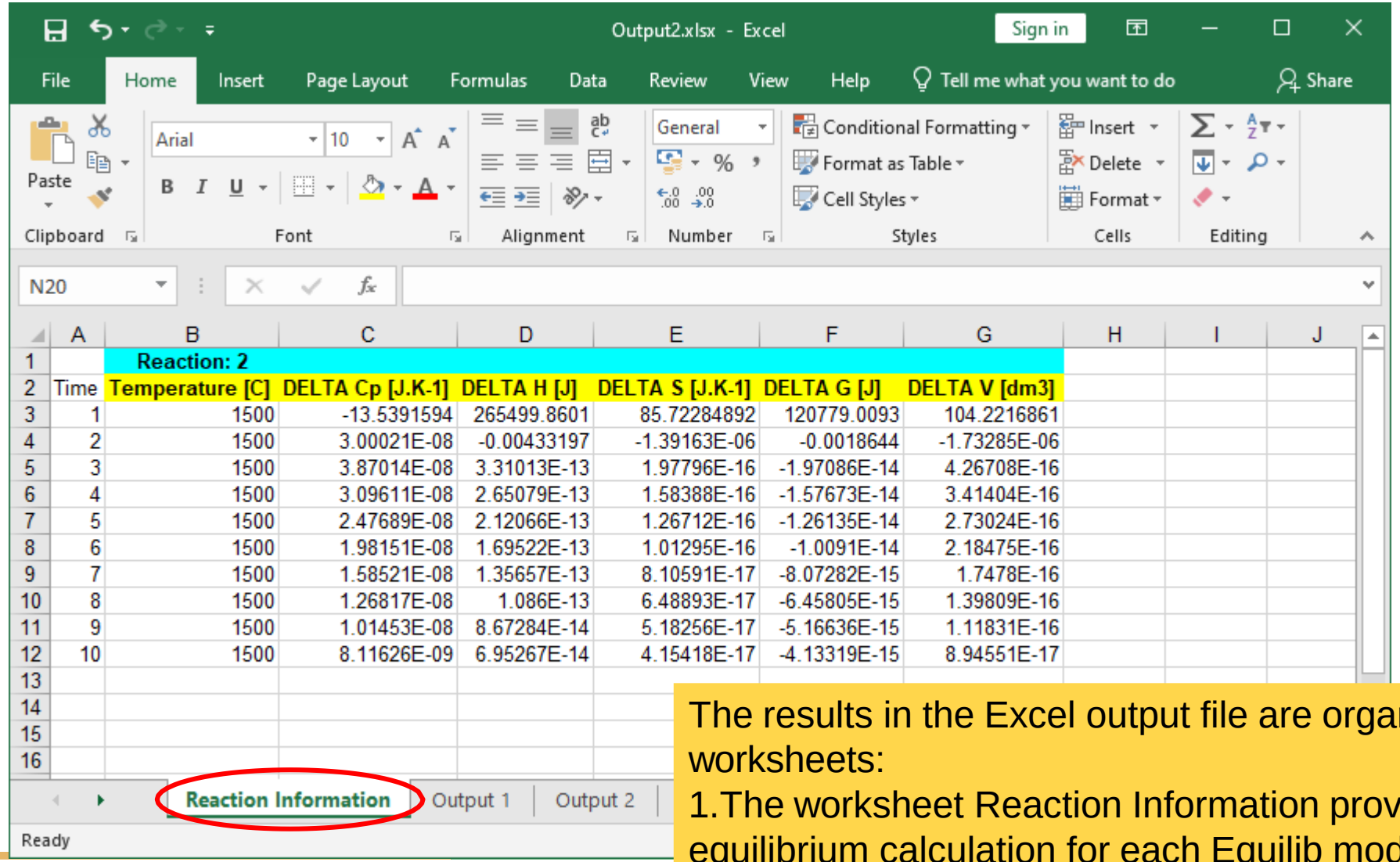
  - Save and load an existing flowsheet
- Step 3: Check the modules – The Initializer
- Step 4: Run the process flowsheet
- **Step 5: View the Results (Output Excel File)**

Step 5: View the results – Excel Output file

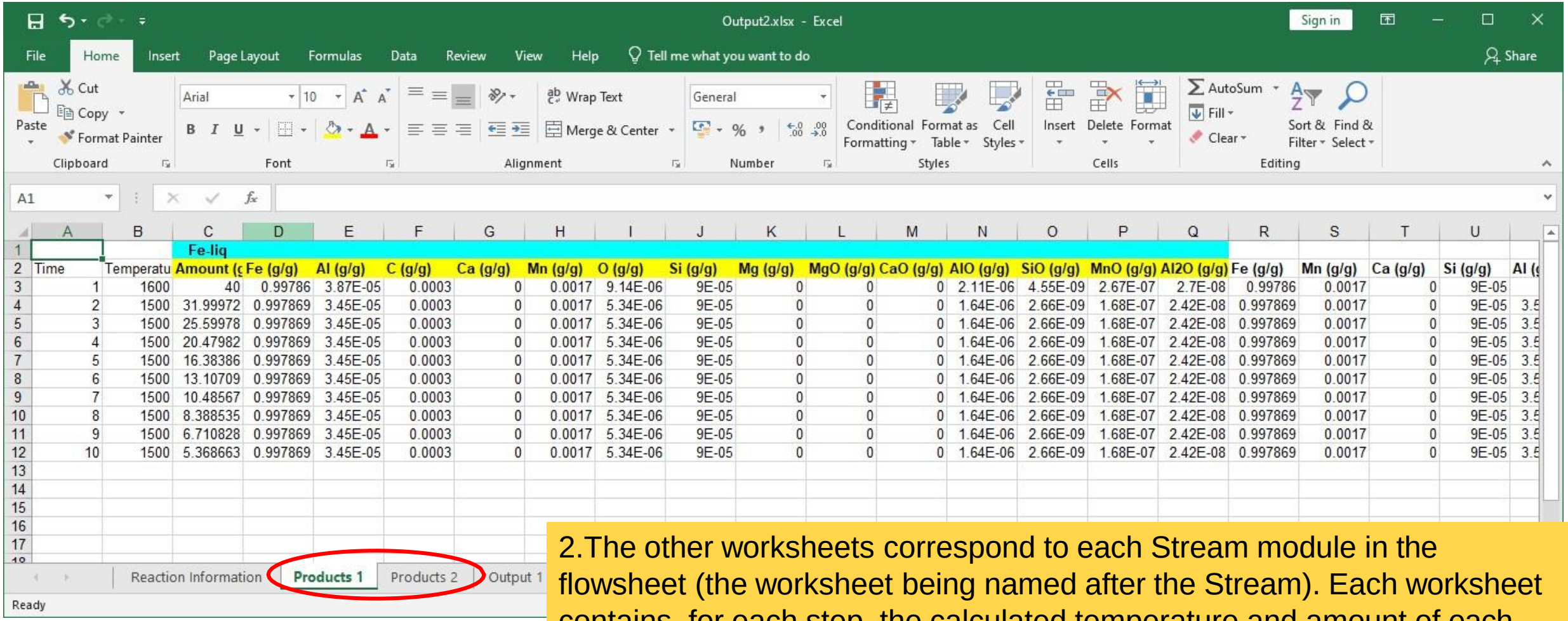


	A	B	C	D	E	F	G
1		Reaction: 2					
2	Time	Temperature [C]	DELTA Cp [J.K-1]	DELTA H [J]	DELTA S [J.K-1]	DELTA G [J]	DELTA V [dm3]
3	1	1500	-13.5391594	265499.8601	85.72284892	120779.0093	104.2216861
4	2	1500	3.00021E-08	-0.00433197	-1.39163E-06	-0.0018644	-1.73285E-06
5	3	1500	3.87014E-08	3.31013E-13	1.97796E-16	-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							

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)



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)