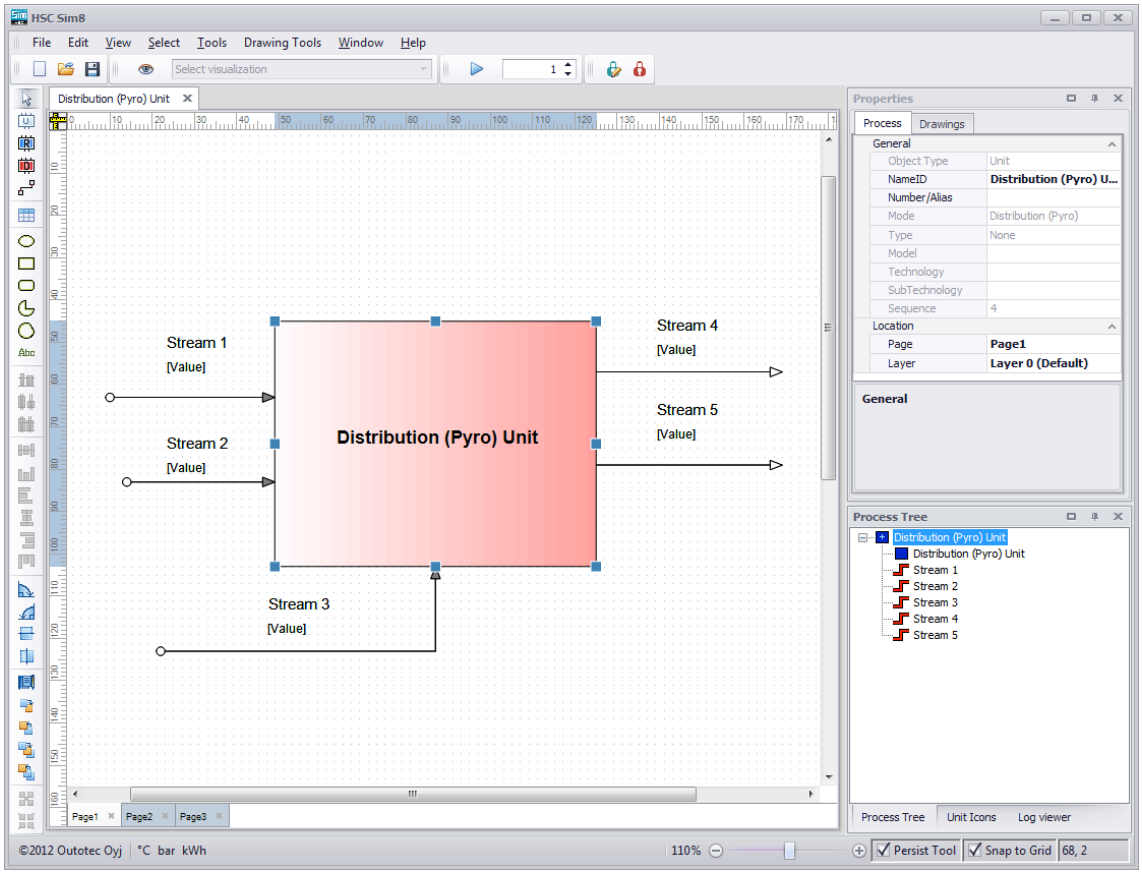
41. Sim Distribution (Pyro) Units



The Distribution unit, also known as the Pyro unit, is a basic unit type in which output species are formed based on the element distribution. This distribution can be defined manually, and regulated further with controls. The Distribution unit also offers Mixer and Equilibrium wizards which allow you to produce the output species without defining the element distribution.

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41.1. Steps to Successful Sim Distribution Simulation

It is important to add the necessary information before simulation can be started. It is good to follow this list while making your Sim Distribution models. Steps 2 to 5 are explained in more detail here.

1. Draw units and streams
2. Specify input streams
3. Specify output streams
4. Specify distribution
5. Set controls
6. Save process
7. Run process

41.2. Specify Input Streams

The unit editor for a distribution unit is shown in **Fig. 1**. Information about the input streams is specified on the Input sheet. The data of the streams are presented in rows. For the input streams, you should specify: the total amount of the stream, the measurement unit for the total amount, temperature, pressure, species, and composition.

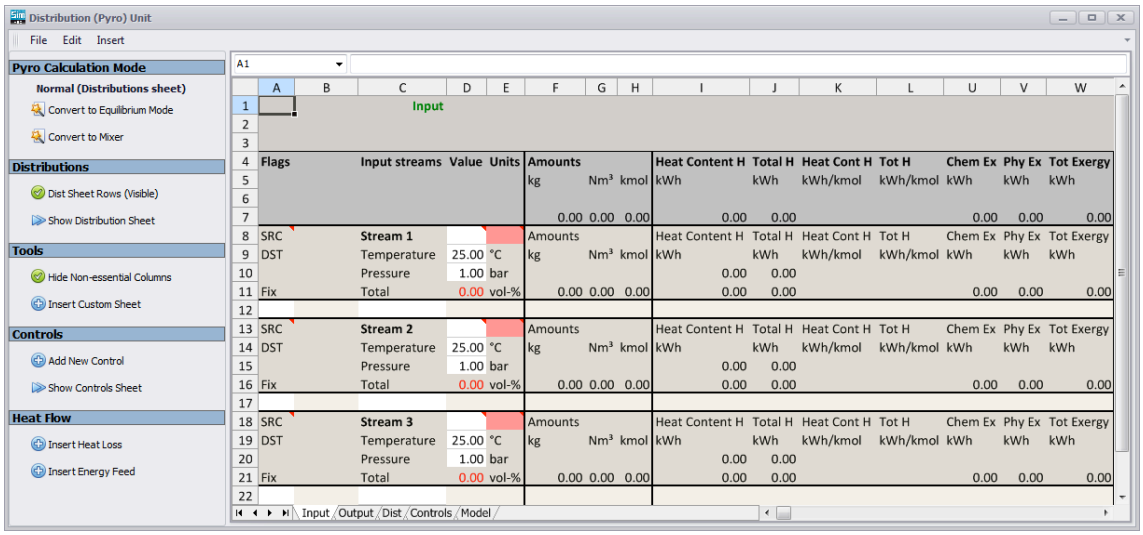

Fig. 1. Distribution unit editor.

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41.2.1. Total Amount, Temperature and Pressure

The total amount of the input stream is specified in the cell next to the stream name (**Fig. 2**). The measurement unit for the total amount is set next to the total amount value (**Fig. 3**). Please note that the selected measurement unit (t/h, kg/h or Nm^3/h) will determine the composition percentage unit (wt % or vol %).

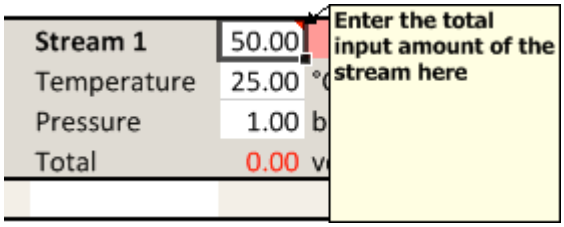

Fig. 2. Total amount of the stream.

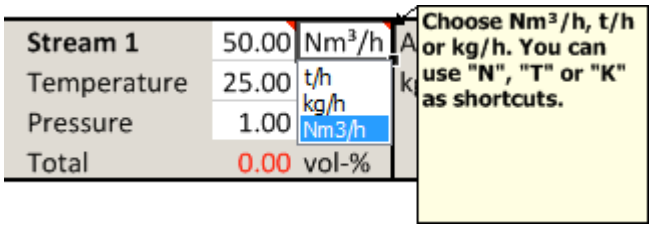

Fig. 3. Measurement unit for the total amount.

The temperature and pressure values can be changed from the cells below the total amount (**Fig. 4**).

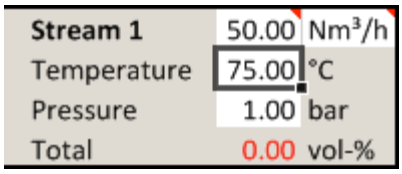

Fig. 4. Temperature and pressure of the stream.

41.2.2. Species and Composition

The species of the stream are entered in the white cells below the stream's header rows (**Fig. 5**).

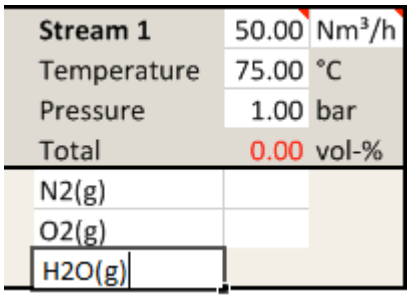

Fig. 5. Enter species in the streams.

Once all the species have been entered, then the composition can be specified (**Fig. 6**). Please pay attention to the composition percentage units.

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Stream 1	50.00	Nm³/h
Temperature	75.00	°C
Pressure	1.00	bar
Total	100.00	vol-%
N2(g)	75.00	
O2(g)	20.00	
H2O(g)	5.00	

Fig. 6. Composition of a stream.

The above steps need to be repeated for all of the input streams which act as raw material inputs. If an input stream is not a raw material input but a stream from another unit, then the properties of this stream cannot be edited on the Input sheet of the destination unit. The energy feeds (or heat losses) can be entered in the streams using the buttons in the left-hand panel (**Fig. 7**).

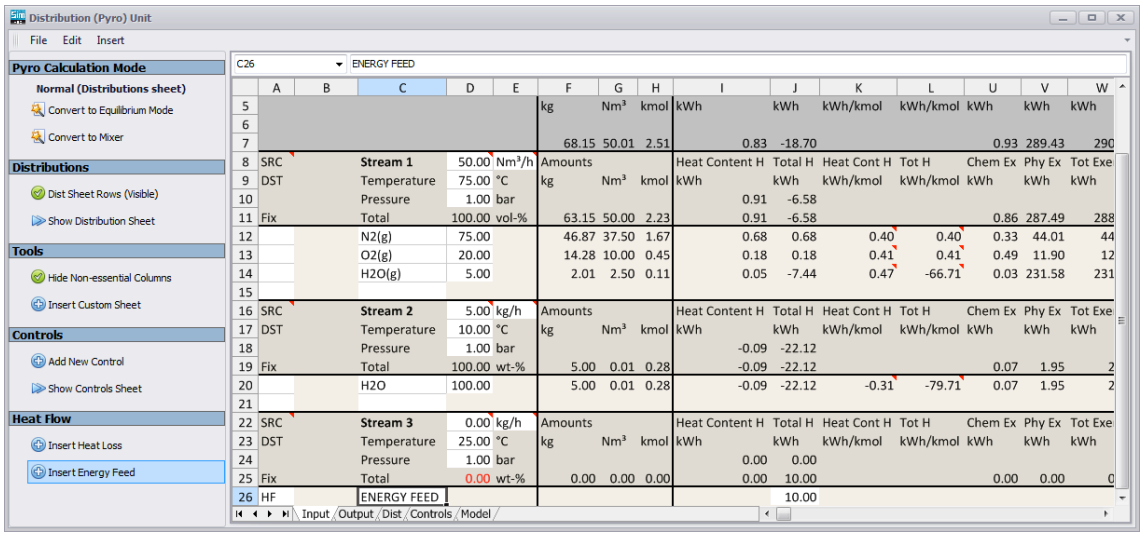

Fig. 7. Inserting an energy feed into a stream.

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41.3. Specify Output Streams

On the Output sheet, the same steps need to be carried out as those done for the Input sheet, with the exception of specifying the total amounts and the stream compositions (**Fig. 8**). The amounts and compositions of the output streams are usually specified on the Dist sheet, but there are also wizards which can be used to specify these properties. Specifying the distribution is introduced in section 41.4.

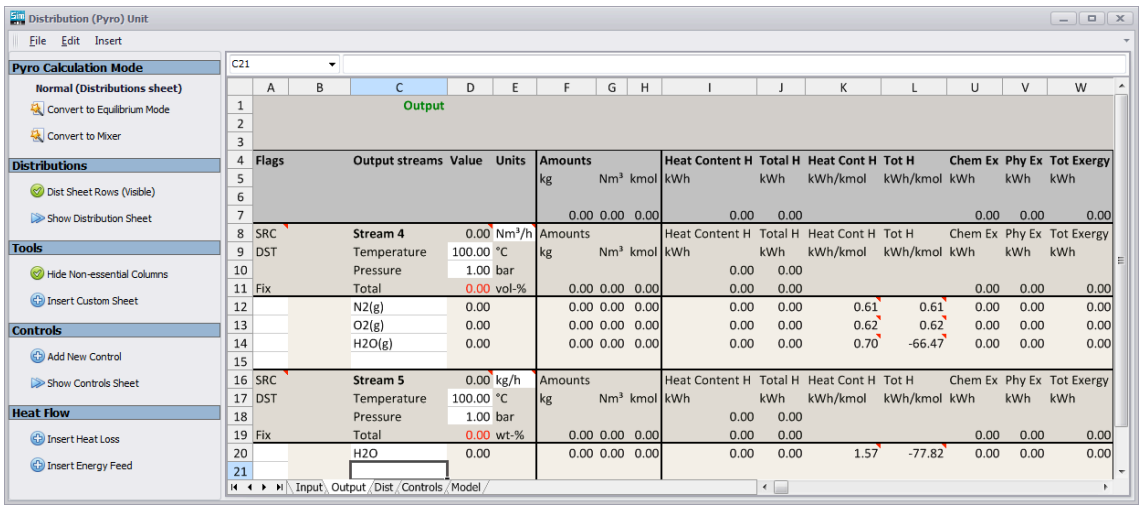

Fig. 8. The user needs to specify: the measurement unit for the amounts, temperature, pressure, and the species for the output streams.

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41.4. Specify Distribution

The distribution of the elements from the Input sheet to the Output sheets can be done by using the Dist sheet or by using the Mixer or Equilibrium wizards.

41.4.1. Dist Sheet

You can create the distribution manually by filling the Dist sheet, which is synchronized with the Output sheet. The elements need to be distributed to the streams and the species within those streams. Therefore, the common approach is to first distribute the elements to streams, and then to species. For instance, in this example, the elements H, N and O need to be distributed to two streams. The first stream contains gaseous species (N2(g), O2(g) and H2O(g)) and the second stream contains pure water (H2O) (**Fig. 9**).

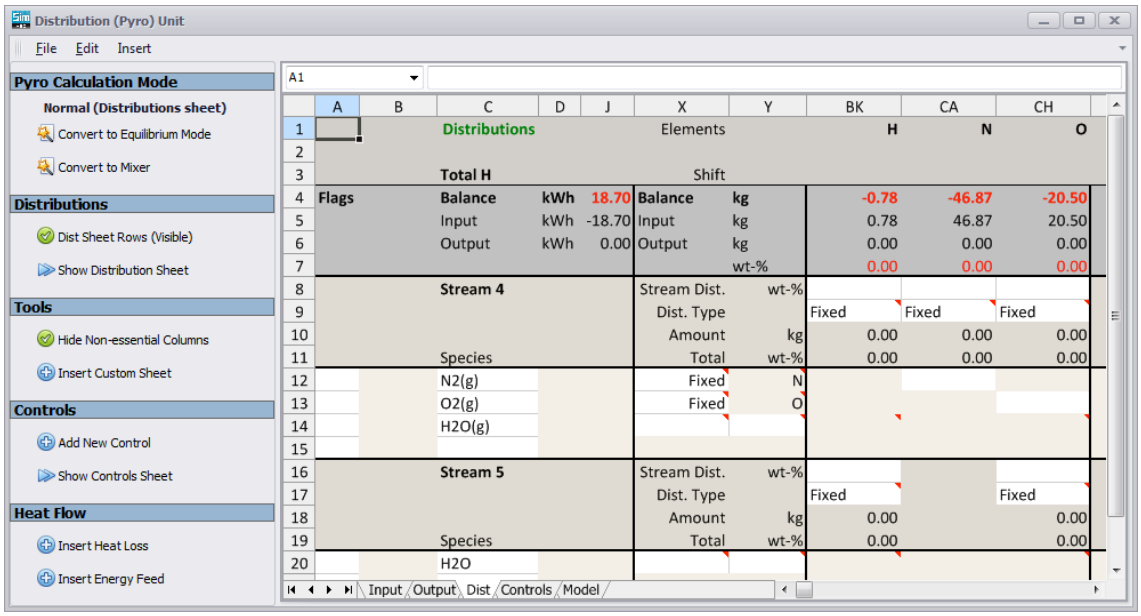

Fig. 9. Dist sheet.

The types of distribution of elements to streams can be Fixed, Rest, and Float:

Fixed - Constant or function value is used.
Rest - All the rest of the element goes into this stream.
Float - Automatically fixed by other elements.

In this example, all the nitrogen is distributed to the first stream and hydrogen and oxygen are distributed to both streams. For instance, it can be initially set that 60% of hydrogen is distributed to the first stream and the rest to the second stream. For oxygen, the distribution type in the second stream will be set as "Float" and "Rest" in the first stream (**Fig. 10**).

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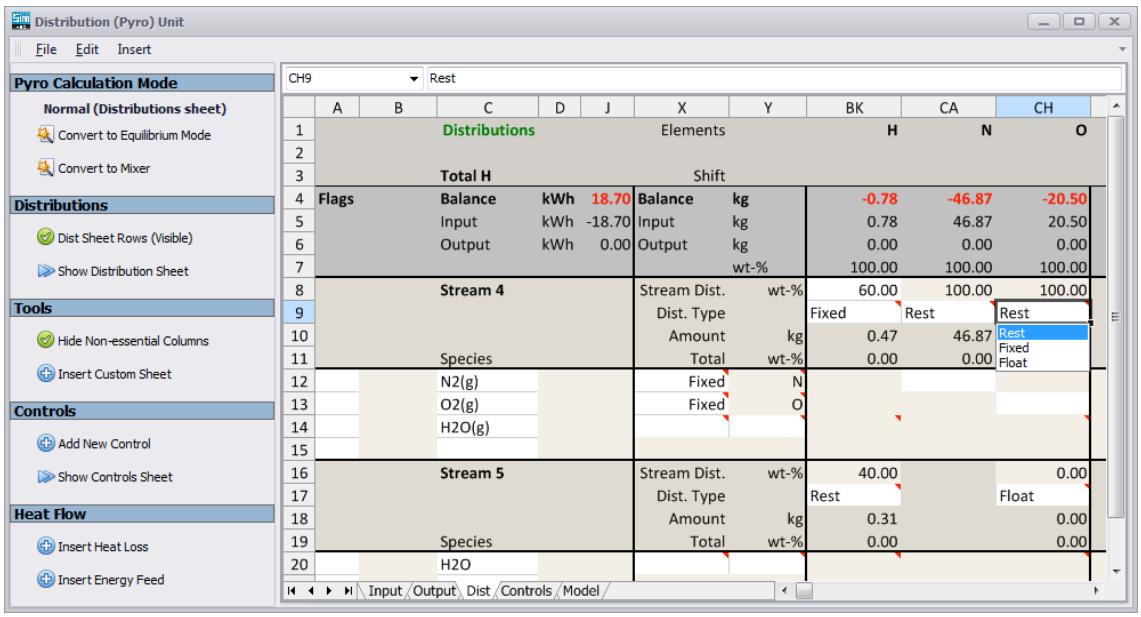

Fig. 10. Distribution of elements to streams.

Next, the elements in the streams will be distributed to the available species. All the species within a stream need to be assigned an element in column Y and a "Fixed" or "Rest" value in column X, which shows how the element amount is distributed to the species.

In this example, H2O can be assigned with all of the hydrogen distributed to the second stream. For the stream with gaseous species, all of the nitrogen will be distributed to the N2(g), all of the hydrogen to the H2O(g), and the remaining oxygen to the O2(g) (**Fig. 11**).

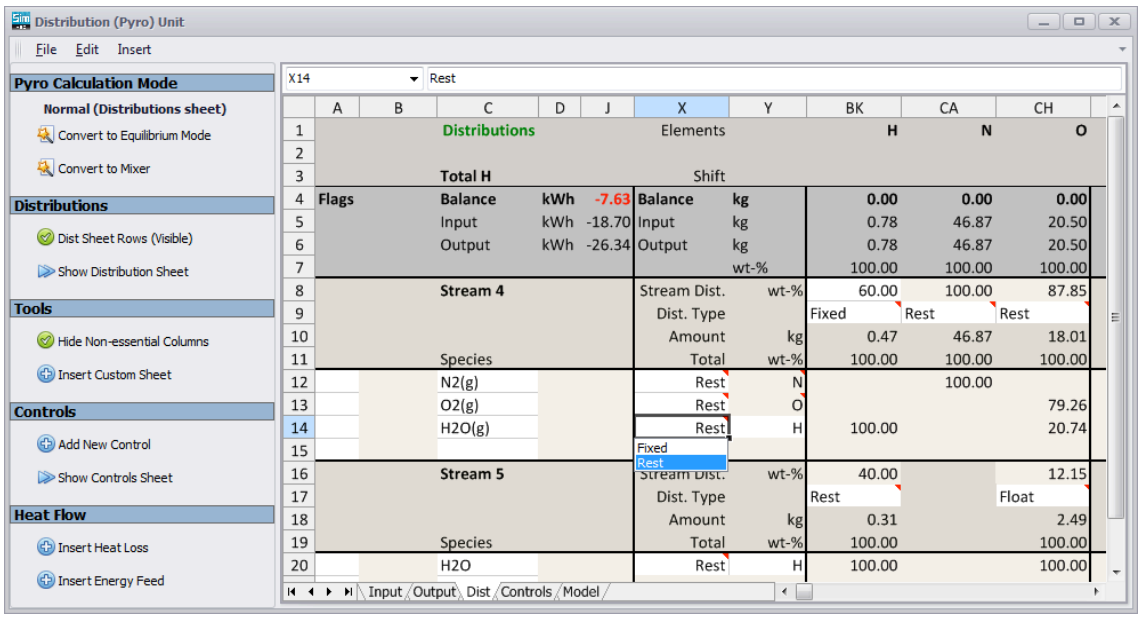

Fig. 11. Elements distributed to species.

NB! When all the elements have been correctly distributed to the species, the element balance, on row 4, should show zero values for all the elements. This ensures that all the atoms are conserved in the distribution unit.

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41.4.2. Mixer Wizard

If the unit operation does not include any reactions between the species, then the species can be distributed directly to the output streams with the Mixer wizard. For the Mixer wizard, you do not need to specify the species for the Output sheet, but you need to specify the measurement unit for the amounts. Please also note that the Mixer wizard requires that the same measurement unit is used for all the streams (both input and output).

The Mixer wizard option is found on the left-hand panel (**Fig. 12**). Distribution in the wizard is specified using percentages for each of the output streams (**Fig. 13**).

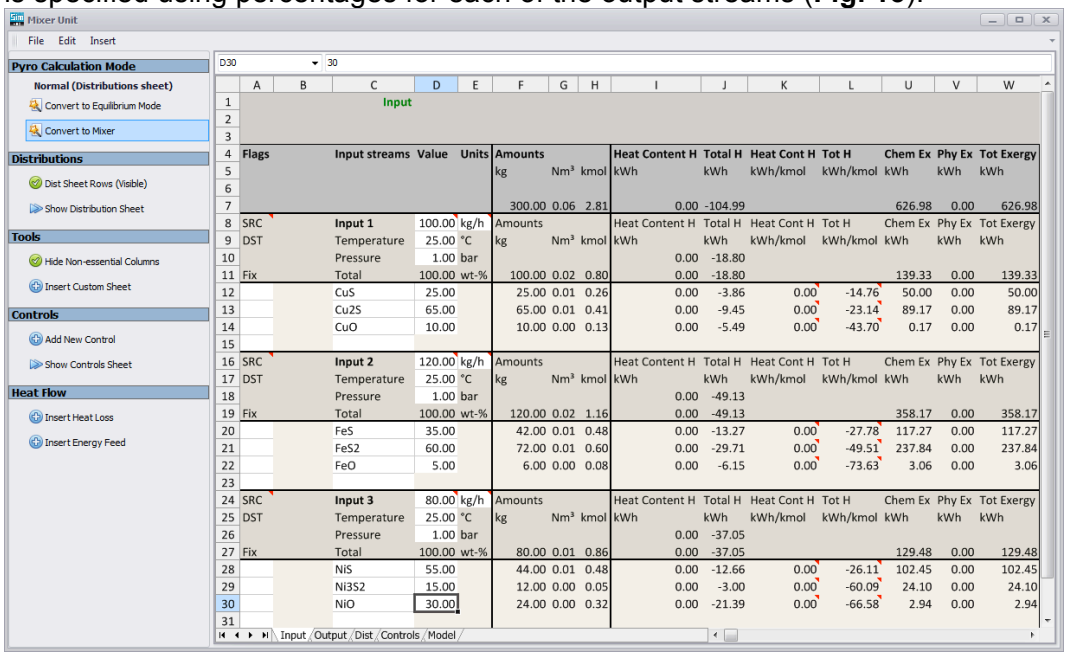

Fig. 12. Using the Mixer wizard.

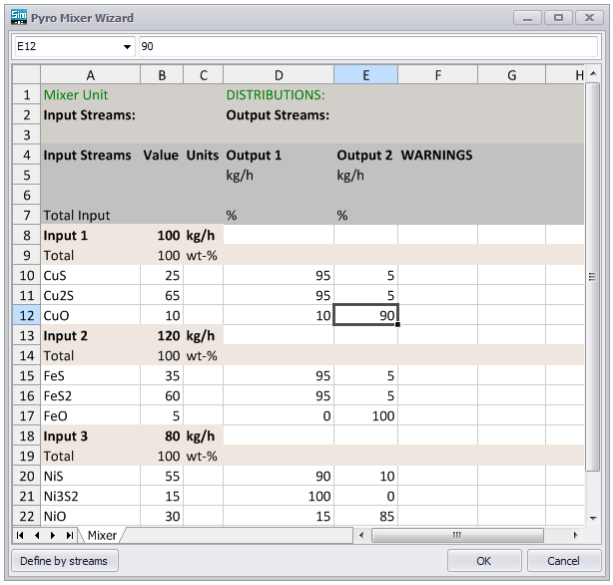

Fig. 13. Distributing species with the Mixer wizard.

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41.4.3. Equilibrium Wizard

The composition of output streams can also be calculated with the Equilibrium wizard. This allows you to distribute the elements from the input sheet to species in the Output streams, based on their chemical stability at the specified output temperature.

The Equilibrium wizard option is found on the left-hand panel (**Fig. 14**) and the equilibrium results are presented on the Gibbs sheet, which is linked to the Output sheet. You need to specify the Input sheet as well as the Output sheet for the wizard. The streams on the Output sheet are assumed to be separate phases in the equilibrium calculations (**Fig. 15**). Phases can be set either as a mixture or as pure phases.

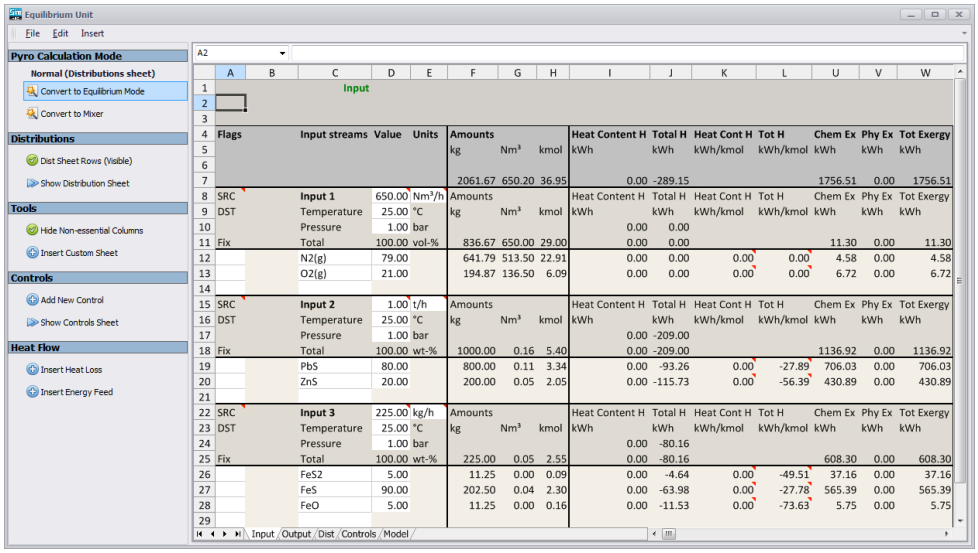

Fig. 14. Using the Equilibrium wizard.

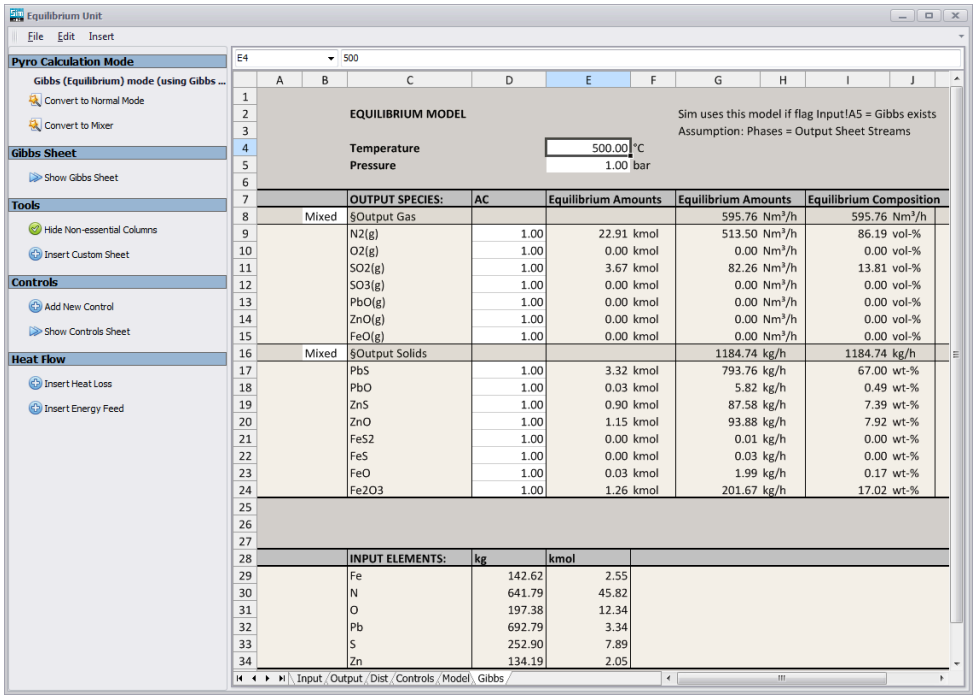

Fig. 15. Distributing elements with the Equilibrium wizard.

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41.5. Set Controls

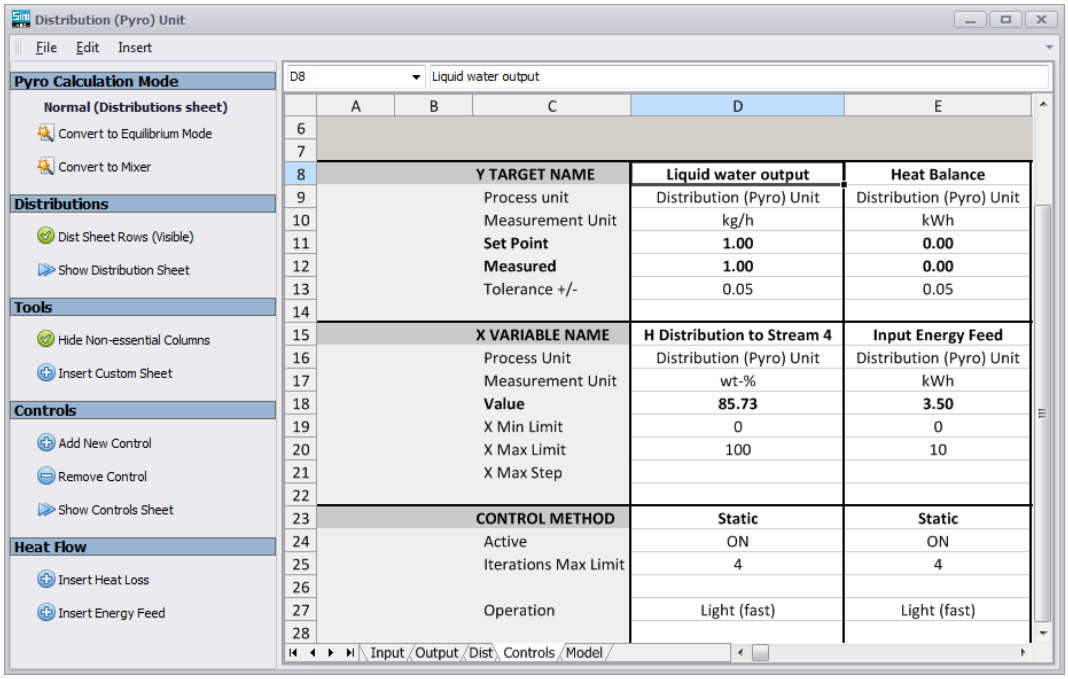

Fig. 16. Controls sheet with two controls.

The HSC Sim Controls sheet makes it possible to create controls that regulate the target parameter cell value using another variable cell value, **Fig. 16**. In principle, Sim Control works exactly like a real process control. For example, in a real process unit you can give a set point to the process unit temperature and regulate the temperature by changing the fuel oil feed.

To create a control on the Controls sheet, you have to set at minimum the Set Point, the Target cell reference, Variable cell reference, the limits for the variable, and the tolerance. You can type this information on the Controls sheet using the following procedure:

1. Type the name and the measurement unit into Controls sheet cells D9 to D10 (optional).
2. Type the Target set value (Set Point) into cell D11.
3. Locate the Target cell in your active unit and right-click "Copy cell reference".
4. Go to Controls sheet cell D12 and right-click "Paste cell reference".
5. Give the tolerance of the calculation in cell D13. When the difference of Set Point and Measured value is smaller than the Tolerance, the control is in balance and will not be calculated further.
6. Type the name and the unit of measure in cells D16 and D17 (optional).
7. Locate the Variable cell in your active unit and select "Copy cell reference".
8. Go to Controls sheet cell D18 and right-click "Paste cell reference".
9. Type **Limit Min** and **Max** in cells D19 and D20, a narrow numerical range speeds up the calculations.

The default **Tolerance** is +/-. A small tolerance increases the calculation time and a large tolerance increases errors. Some 2% of the target value may be a good compromise. The control will not be taken into account if the value is within the tolerance.

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Sim Controls have exactly the same **limitations** as real process controls, for example:

- If the target cell does not depend on the variable cell value, the iterations will fail.
- If an external variable cell is used, there may be a long delay before the effect on the target value becomes visible. In these cases a lot of iteration rounds might be needed to reach the Set Point. This increases the calculation time.

Table 1. Information on the Controls sheet.

Row	Name	Description
8	Y Target Name	Name of Y (optional)
9	Process Unit	Unit name (optional)
10	Measurement Unit	Name of the unit of measure (optional)
11	**Set Point**	**Set point of Y (obligatory)**
12	**Measured**	**Y cell reference (obligatory)**
13	**Tolerance +/-**	**Y tolerance (obligatory**)
15	X Variable Name	Name of X (optional)
16	Process Unit	Unit name (optional)
17	Measurement Unit	Name of the unit of measure (optional)
18	**Value**	**X cell reference (obligatory)**
19	**X Min Limit**	**Min limit of the X range (obligatory)**
20	**X Max Limit**	**Max limit of the X range (obligatory)**
21	X Max Step	Maximum X Step (optional, default = empty)
23	Control Method	Iteration method (optional, default = Auto[1])
24	Active	Set control ON/OFF (optional, default = empty = ON)
25	Iterations max limit	Max number of iterations (optional, default = 10)
26	Iterations min limit	Min number of iterations (optional, default = empty)
27	Operation	Control calculation operation (optional, default = Light[2])

[1]**Auto** (Solves the control with information on rows 24 - 27), **Auto Smart** (Same as Auto except changes X Max Step and Iterations max limit when needed), **PID** (not in use, will be added to the HSC8 version).

[2]**Light** (Solves the control with modified tangent method, fast), **Robust** (Solves the control with modified Newton method, slow), **Simple direct** (Increases X value when Measured value is too small. The step used can be specified in X max step.), **Simple reverse** (Decreases X value when Measured value is too small. The step used can be specified in X max step.).

41.5.1. Internal and External Controls

1. Internal control in which the target and variable cells exist in the same process unit (FAST).

2. External control in which the target and variable cells exist in different process units (SLOW).

Calculation of an internal control is fast because only one unit is calculated. Usually you can create a large number of **internal controls** in a process without a dramatic drop in calculation speed, because they do not increase the number of calculation rounds of the process.

Calculation of an external control might take more time because material must be recirculated within the whole process several times to reach a stable target value. Usually only a few **external controls** can be used in one process without a considerable decrease in the calculation speed, because external controls might multiply the calculation rounds of the process.

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41.5.2. Advice When Using Controls

- It is recommended to moderate large changes of the variable with the use of **X Max Step**, when using external controls with slow responses.
- The **RecoveryX** add-in function cannot be used in the Target cell, because it is recalculated only after all the calculation rounds have been completed.
- The large number of thermochemical add-in functions (**StreamH**, **StreamS**, etc.) may reduce the calculation speed if the argument value changes in each control iteration round, because the data search from the H, S, and Cp database takes time. Use these add-in functions only when necessary.

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