42. Sim Distribution Example

Magnetite Oxidation Example

Pelletized magnetite (Fe_3O_4) ore can be oxidized to hematite (Fe_2O_3) in a shaft furnace. The typical magnetite content of the ore is approx. 95%. Oxidation is usually done by feeding air into the shaft furnace. Some excess oxygen is needed to complete the reaction; the free oxygen in process gas is usually approx. 5%. About 1% of the iron does not react. Coal is used as a fuel to keep the product temperature at 700 °C.

This kind of unit process can be controlled by air and coal feeds. The ore feed can be fixed to approx. 200 t/h. Now, please create a process model of the shaft furnace with oxygen and coal controls.

Walkthrough steps:

1. Draw the flowsheet
2. Draw the streams on the flowsheet
3. Rename the units and streams
4. Save the process
5. Specify the raw material streams
6. Specify the output streams
7. Create a model
    a. Distribution to output streams
    b. Distribution to species within streams
8. Create the controls
9. Run the process model

42.1. Step 1. Draw the flowsheet

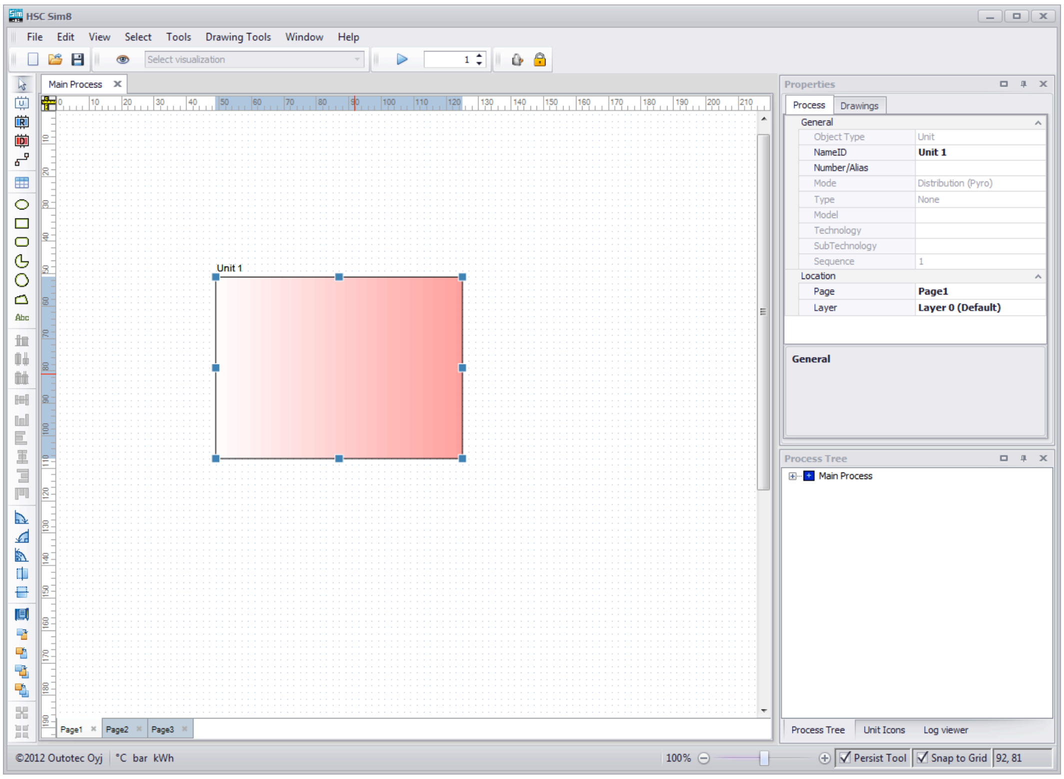

Fig. 1. Draw unit (distribution) on the flowsheet.

First, draw the flowsheet for the process. Usually it is easiest to start with the units of the process (**Fig. 1**). You can draw a generic unit and select its model from the Unit Model Editor, or simply draw a distribution unit by using the red unit icon.

42.2. Step 2. Draw the Streams on the Flowsheet

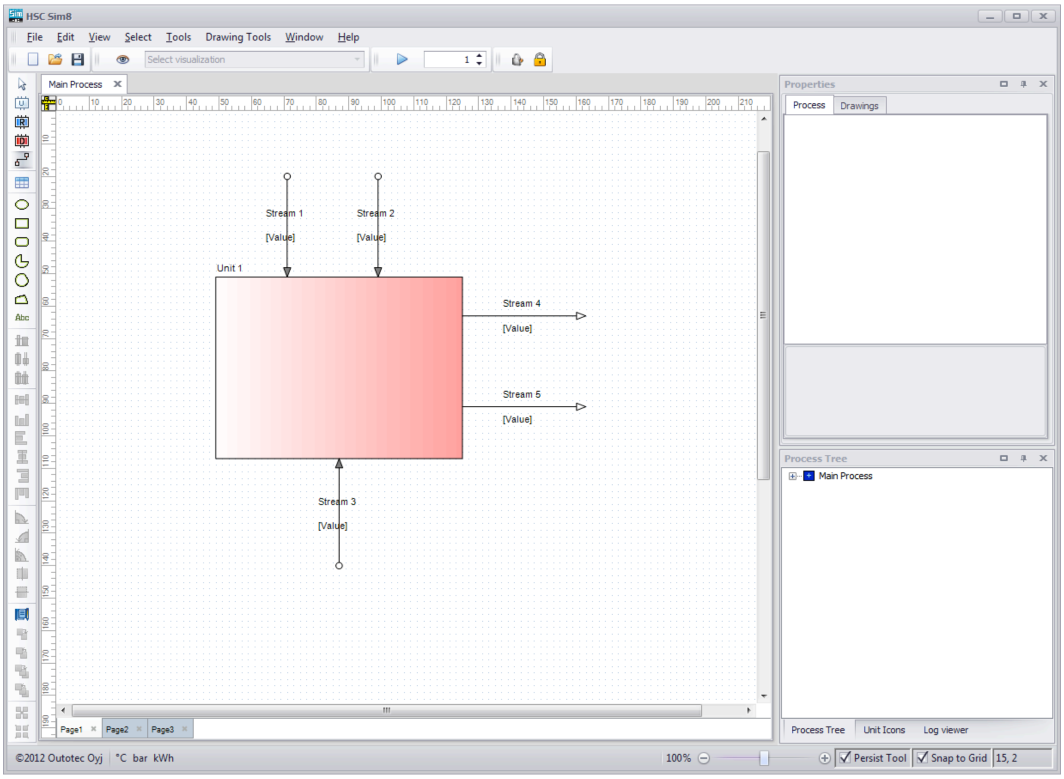

Fig. 2. Draw streams on the flowsheet.

The second step is to draw streams (**Fig. 2**), which must be done using the Stream tool on the left toolbar. The shapes and colors at the end points of the streams indicate their connections. You can also check the Source and Destination units for each stream from the Process tab. If a stream is not connected from either end, then this value is shown as a question mark (?) for the missing Source or Destination value.

Process raw material streams do not have specified Sources, whereas the Destination units are missing for the process output streams. Intermediate streams should have both Source and Destination values specified.

42.3. Step 3. Rename the Units and Streams

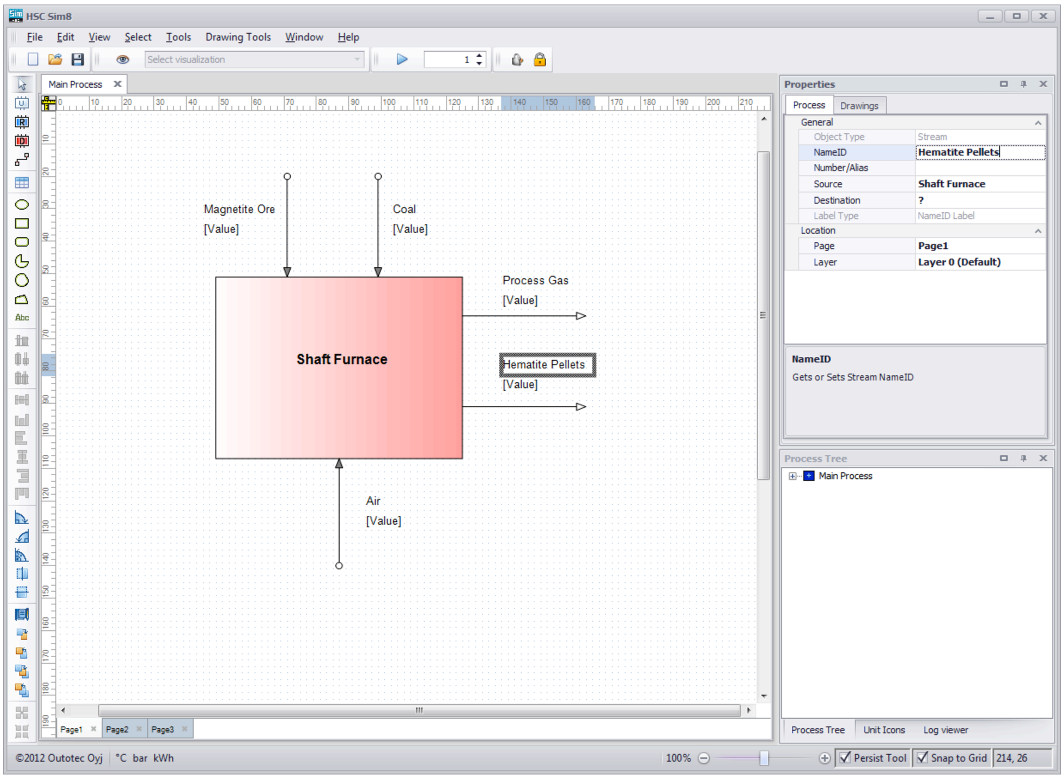

Fig. 3. Renaming units and streams makes flowsheet easier to read.

You can relocate the unit and stream name labels by dragging them with the mouse. Select the unit or stream and rename it using the NameID property. This property is used to identify unit and stream objects. Please use short and illustrative names.

The Drawings tab lets you change the label text formatting. Formatting options can be applied to the labels one by one, or you can select multiple labels and change the formatting for all of them. The Select menu at the top bar offers options to select all certain types of labels from the flowsheet.

42.4. Step 4. Save the Process

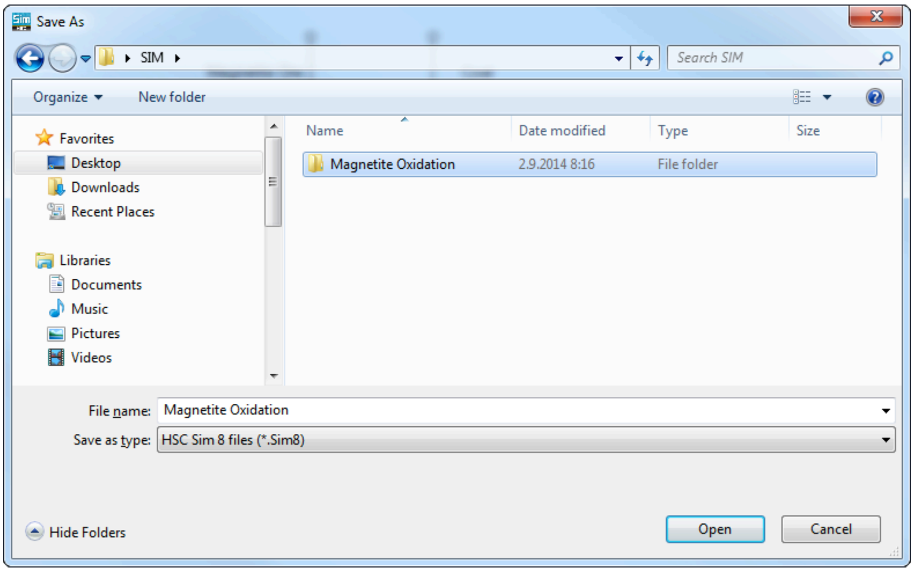

Fig. 4. A process has to have a folder of its own.

It is better to save the process too often rather than too seldom, because a saved process allows you to recover the earlier design stage in case of user or computer errors.

It is necessary to create a separate file folder for each process using the Create New Folder tool, see **Fig. 4**. The process name is also the most logical name for the file folder. In this case the folder name is Magnetite Oxidation and the process name is Magnetite Oxidation. A process can consist of several files and all of these files will be saved into this same folder.

42.5. Step 5. Specify the Raw Material Streams

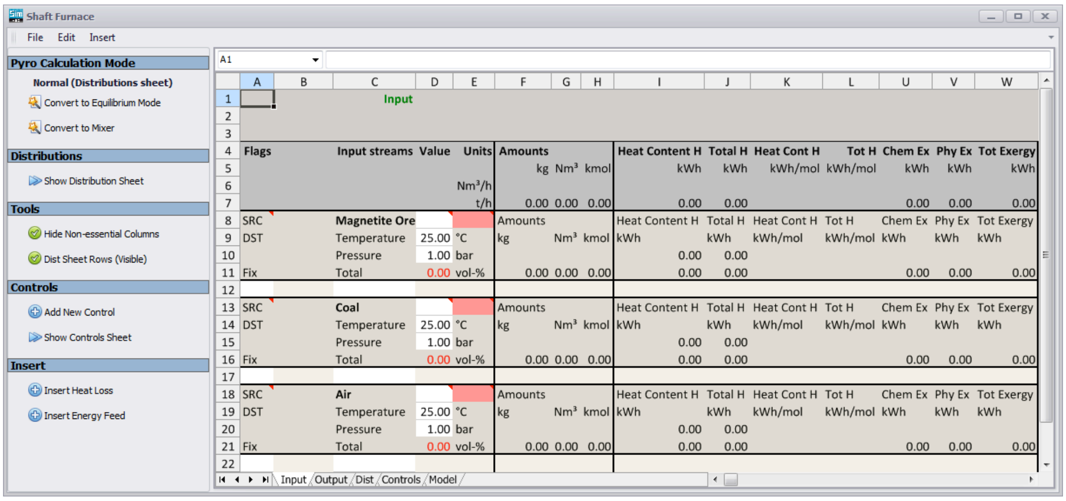

Fig. 5. Raw materials on the Input sheet.

You can open Unit Editor by double-clicking the unit icon on the flowsheet. The raw material streams can be found on the Input sheet. At the beginning these streams are empty. Species can be typed into streams manually.

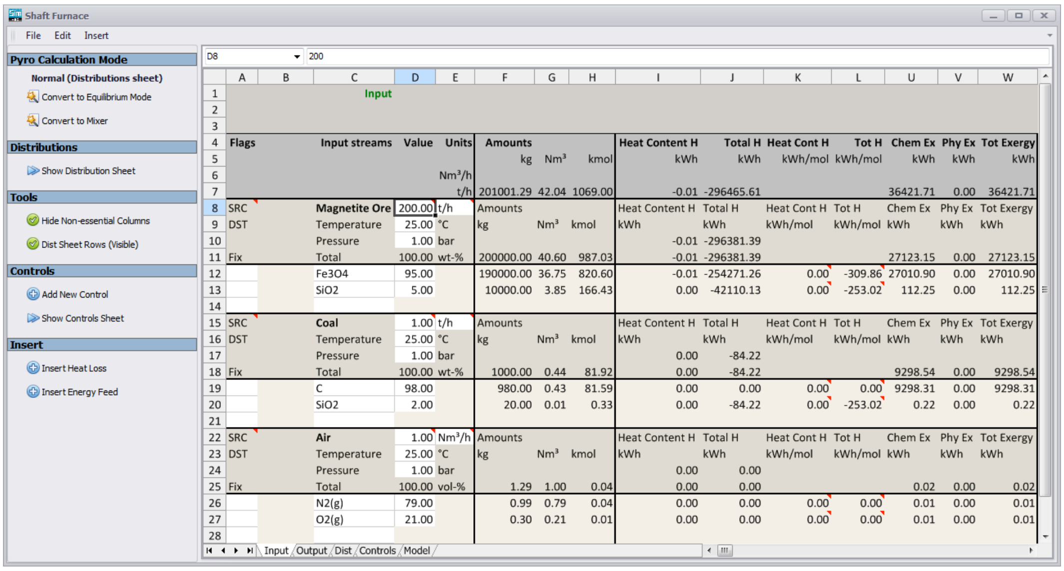

Fig. 6. Specify stream species, compositions, raw material amounts and measure units.

You need to specify the raw material stream species as well as their compositions and temperatures. It is also important to specify the measure units for the streams. Valid selections are:

- t/h
- kg/h
- Nm3/h (only for gases)

Please note that the stream composition is given in wt-%, if mass units are used, and in vol-%, if normal cubic meters are used. If the feed amount is not yet available then it is good to specify an initial value such as 1 t/h, especially if this raw material will be used within some control.

42.6. Step 6. Specify the Output Streams

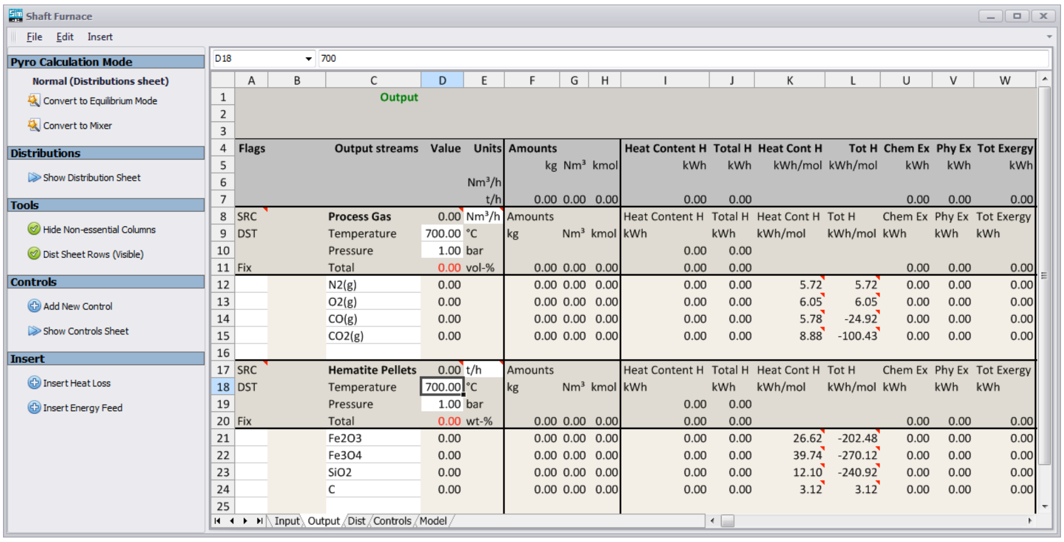

Fig. 7. Output streams are specified on the Output sheet.

You need to specify the species, temperatures, and the measure units of the output streams. Please note that the output stream amounts and species distributions cannot be edited manually, as they will be calculated later.

The Output and Dist sheet streams have been synchronized with each other. This means that when you type species on the Output sheet they will also appear on the Dist sheet.

42.7. Step 7. Create A Model

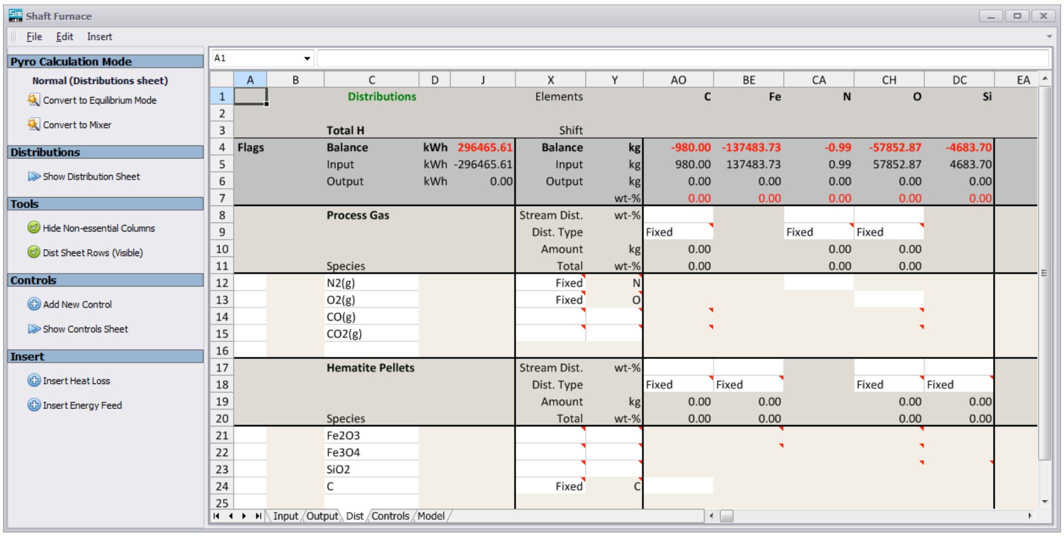

Fig. 8. Element distributions need to be specified on the Dist sheet.

The Sim Distribution mode automatically calculates the total input amounts for the input streams and converts these into elements. The user must specify on the Dist sheet how these elements will be distributed:

a) into output streams
b) into species within one stream

The Popup list tool can be used in the specification procedure. This tool is automatically opened when you click a cell where the operation is possible. The options are:

- **Fixed**
  The distribution is fixed with a constant %-value or an Excel-type formula.
  Only a constant value cell may be used as a variable on the Controls sheet!
- **Rest**
  When all the specifications have been made for a certain element, then the remaining fraction of the element must go to one species and one phase.
- **Float**
  This option means that the current cell has been automatically specified by the other elements like metals. It is usually wise to specify oxygen, sulfur, etc. as floating elements.

42.7.1. Step 7.a - Distribution to Output Streams

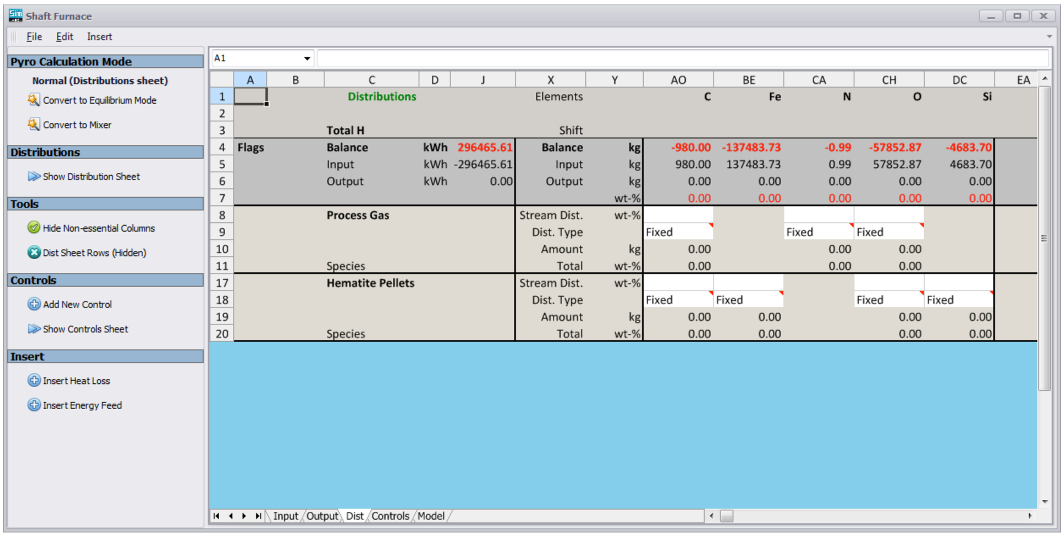

Fig. 9. Distribution to output streams.

When distributing the elements to output streams, it might be helpful to hide the species rows with the "Dist Sheet Rows" button in the left-hand panel (**Fig. 9**).

An easy way to start is to fix the elements which are present only in one stream. In this example, this applies to nitrogen (N), iron (Fe), and silicon (Si). Nitrogen is present only in the "Process Gas" stream, whereas iron and silicon are only found in the "Hematite Pellets" stream. To distribute these elements, set their status to Fixed in the correct streams and give their wt-% value as 100 (**Fig. 10**). Note that you can also use the Rest status for the elements that are found only in one stream.

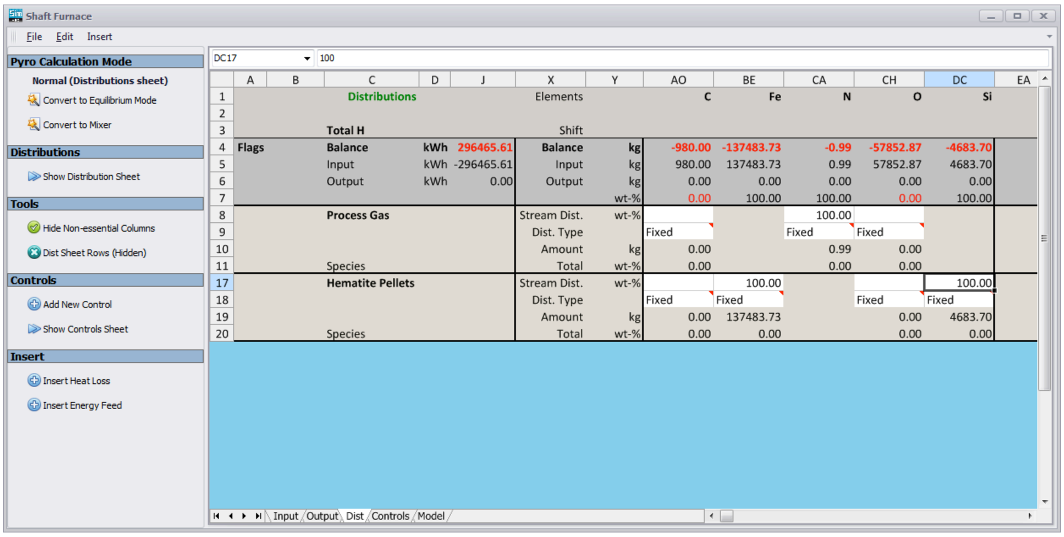

Fig. 10. Fixing elements (N, Fe, and Si) in the output streams.

For elements that are present in several streams, distribution can be done e.g. by fixing a value for one stream and letting the remaining amount go to the other. For example, you can define that 0.1 wt-% of carbon (C) goes into the "Hematite Pellets" stream and the rest will be distributed to the "Process Gas" stream. To do this, set the status of carbon to Fixed in the "Hematite Pellets" stream and give the wt-% value as 0.1, then set the status of carbon in the "Process Gas" stream as Rest (**Fig. 11**).

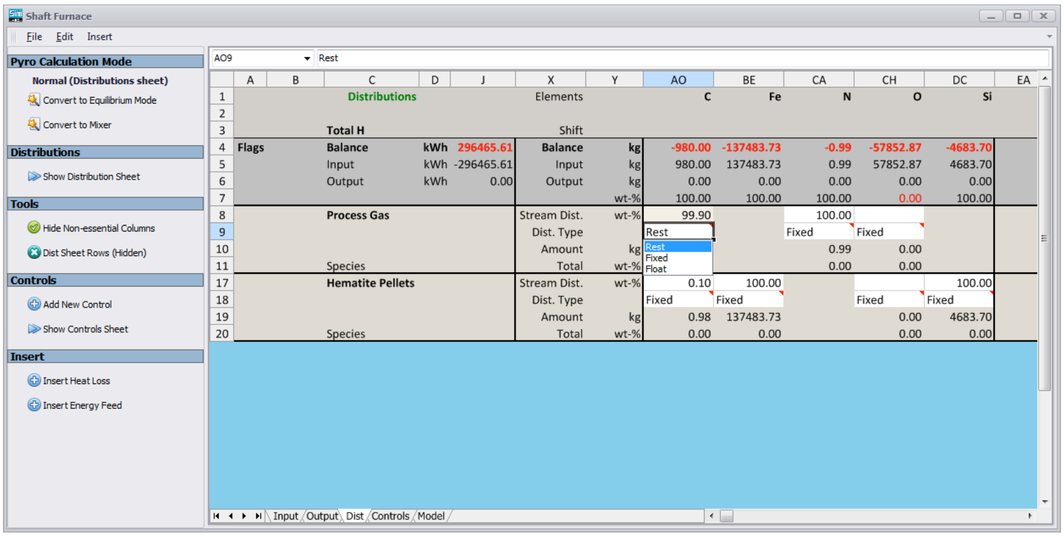

Fig. 11. Fixed fraction of carbon in the pellets stream and rest in the gas stream.

Finally, oxygen needs to be distributed to the output streams. In the "Hematite Pellets" stream, oxygen is present in iron oxides and silica. By letting the iron and silicon content of the pellet stream determine the amount of oxygen, the status can be set as Float. The rest of the oxygen will be distributed to the "Process Gas" stream by setting the status as Rest (**Fig. 12**).

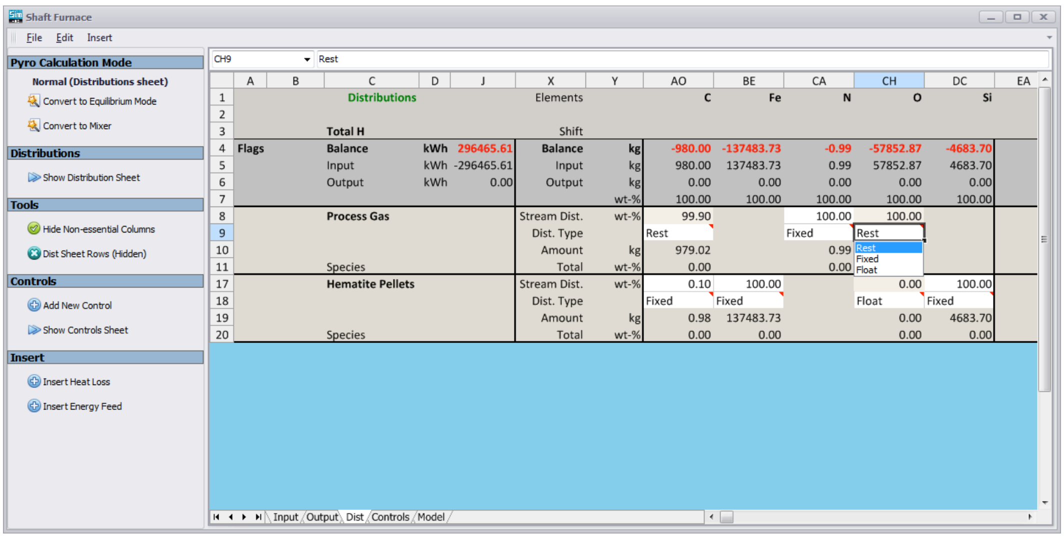

Fig. 12. Distribution of oxygen to output streams.

Please note that after the elemental distribution to the output streams is finished, the wt-% values in row 7 should all be 100.

42.7.2. Step 7.b - Distribution to Species within Streams

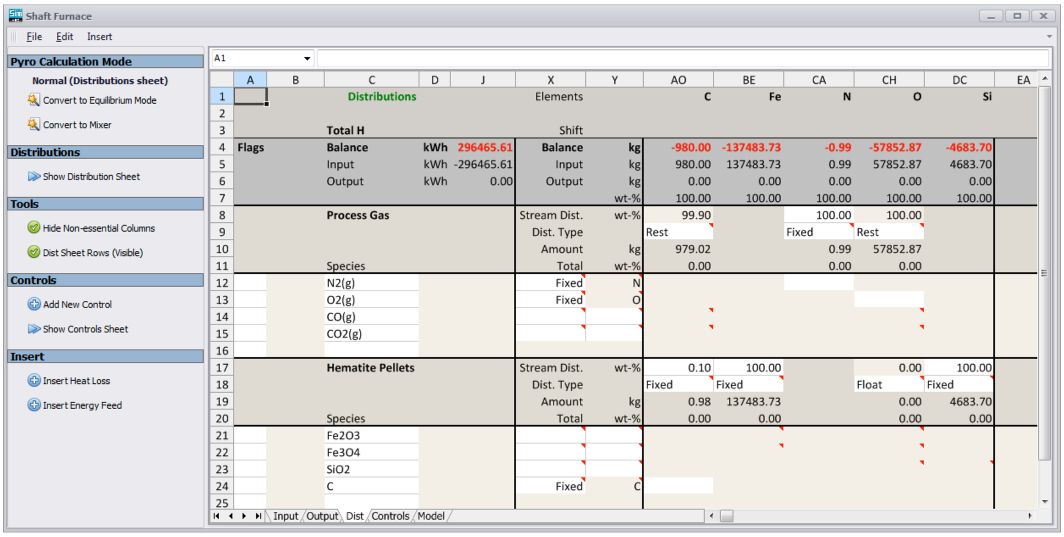

Fig. 13. Distribution of elements to species.

All the species in the streams need to be assigned with an element in column Y and a status in column X. These parameters together are used to distribute the elements to species. Species that contain only a single element have their element assigned automatically.

In the "Hematite Pellets" stream, it is easiest to start with carbon (C) and silica (SiO_2). For carbon atoms, there is only one species (C), so this species can be assigned to contain 100% of the stream's carbon content. Similarly, you can fix the silica amount by assigning the species to the element Si, and setting the species to contain 100% of the stream's silicon content (**Fig. 14**).

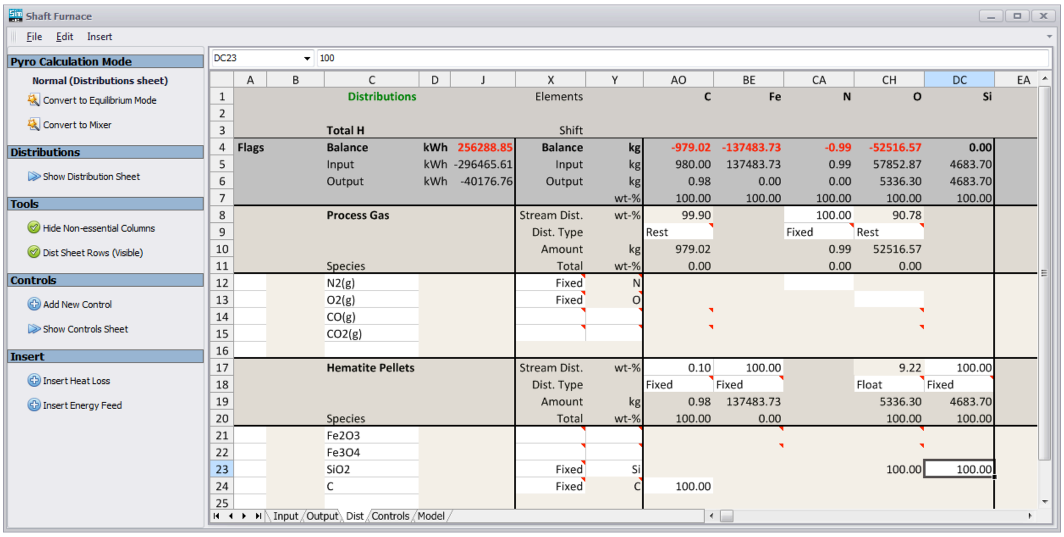

Fig. 14. Carbon and silicon distribution in the pellets stream.

Iron is distributed between magnetite (Fe3O4) and hematite (Fe2O3). In this example, it is assumed that almost all of the magnetite is oxidized. This can be simulated by fixing 1% of stream's iron content to Fe3O4 and distributing the rest to Fe2O3 (**Fig. 15**).

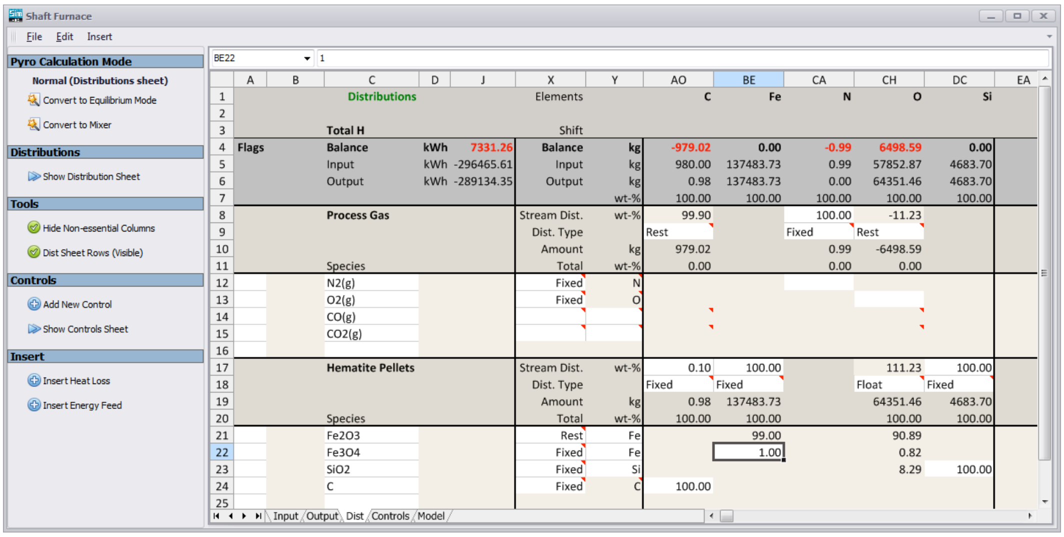

Fig. 15. Iron distribution to the pellets stream.

Next, the elements can be distributed to the "Process Gas" stream. Again, an easy way to start is to distribute the nitrogen (N) atoms to the only species (N2(g)) which contains nitrogen (**Fig. 16**).

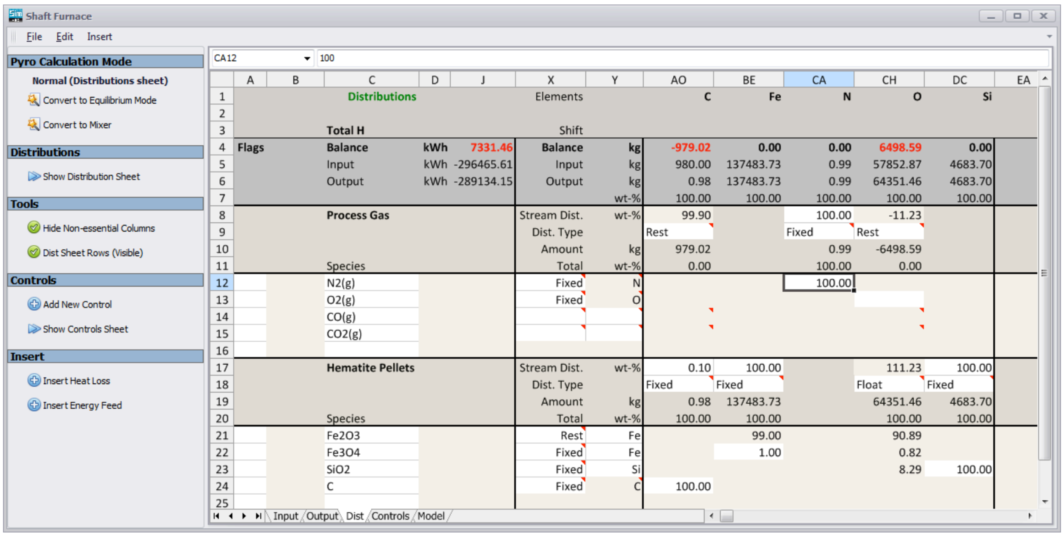

Fig. 16. Nitrogen distribution in the gas stream.

For the carbon-containing species (CO(g) and CO2(g)), it can be assumed that enough oxygen is provided for all of the carbon in the gas stream to be oxidized into carbon dioxide. Thus, carbon (C) can be assigned to both species and the CO(g) will be fixed at 0.00, and for CO2(g) the status can be set as Rest (**Fig. 17**).

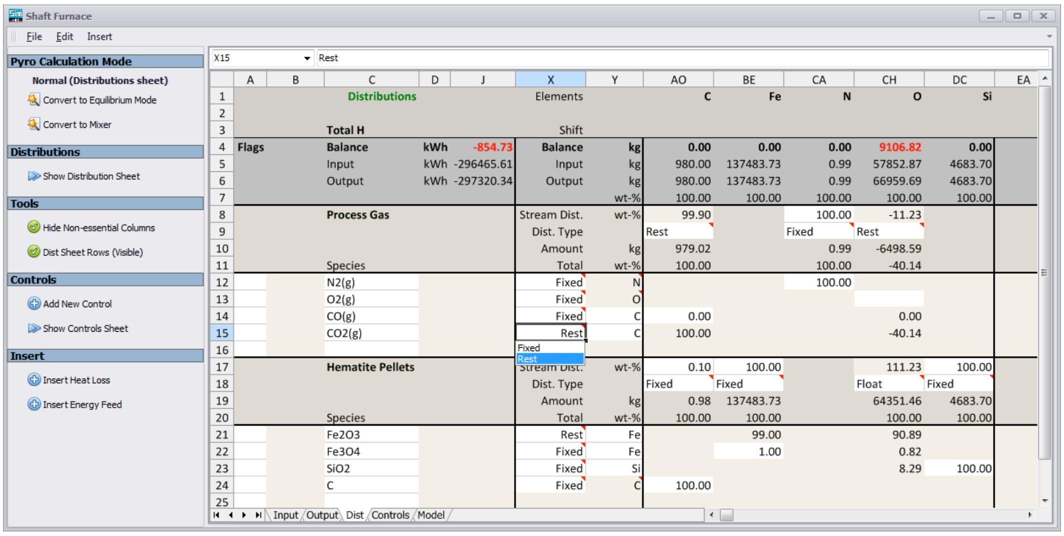

Fig. 17. Carbon distribution in the gas stream.

The final thing to do is to distribute all excess oxygen atoms (O) to oxygen gas (O2(g)). This can be done by setting the status to Rest (**Fig. 18**).

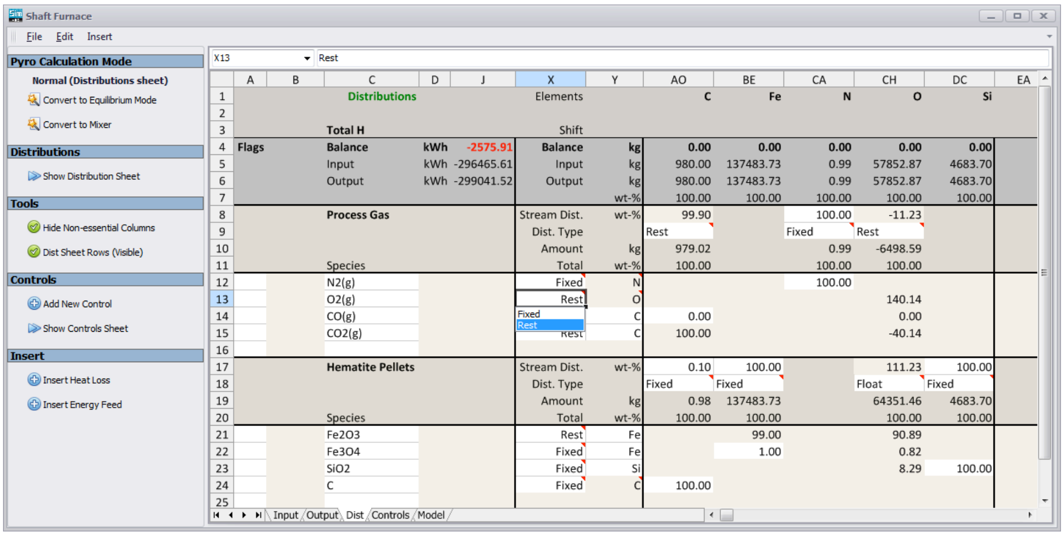

Fig. 18. Oxygen distribution in the gas stream.

Now the distribution of elements in the output streams is ready. It is important to notice that for a correctly filled Dist sheet, the Balance value for all of the elements is equal to zero (**Fig. 19**). This indicates that all the atoms are conserved, and thus the elemental balance is maintained.

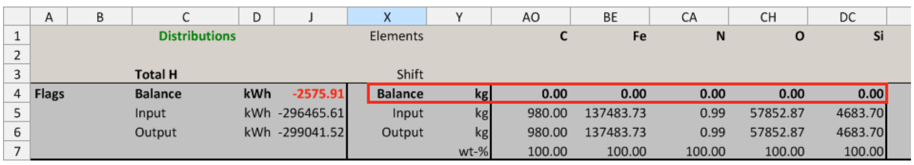

Fig. 19. Zero values indicate that all the atoms are conserved.

42.8. Step 8. Create the Controls

Controls are often used to regulate distribution values, output stream compositions and heat balances. For each control we have to specify:

1) A target cell and a Set Point value for this cell
2) A variable cell used to regulate the target cell

The variable cell must have some effect on the target cell parameter. If this is not true, then the control will not work. The situation is exactly the same when you control real processes and plants.

In this example two controls are used: one to regulate the O2 content in the "Process Gas" stream, and another to ensure that the heat balance is maintained.

First, add two controls to the sheet by clicking the **Add New Control** button in the left-hand panel, and type the name of the first control (**Fig. 20**).

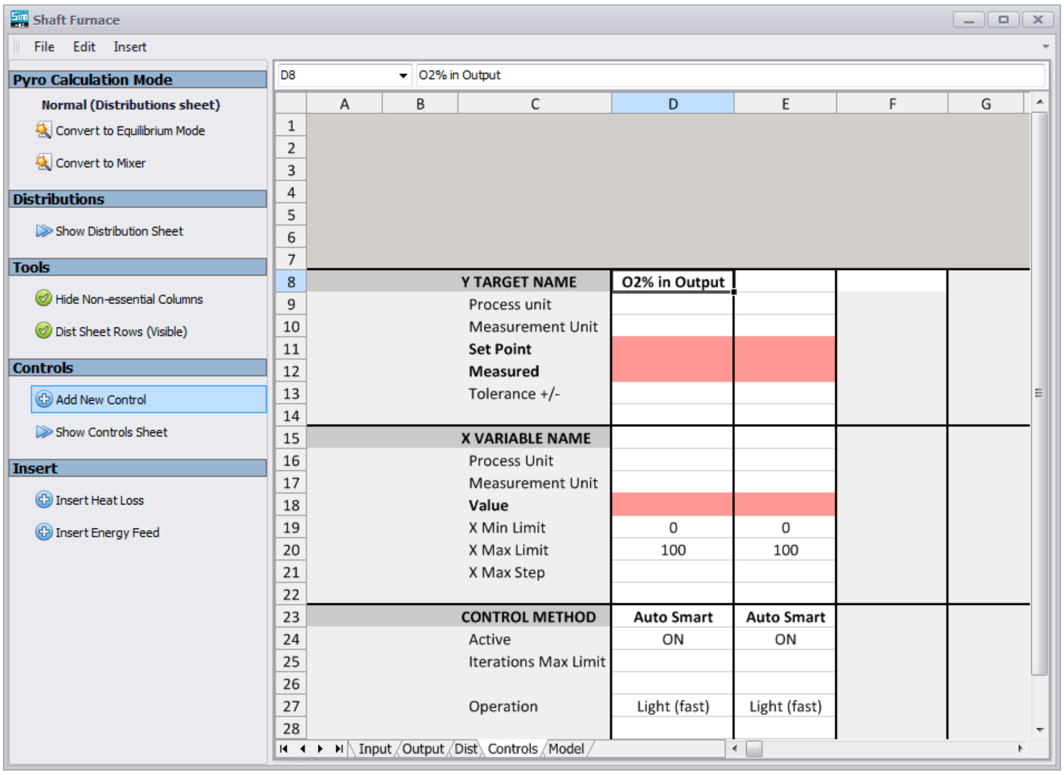

Fig. 20. Controls can be added to the sheet with the Add New Control button.

Next, set the cell reference for the target parameter. For this control, the correct cell can be found on the Output sheet, cell D13 (Output!D13). To set this cell reference, you can go to the Output sheet, right-click the correct cell and select Copy cell reference (**Fig. 21**).

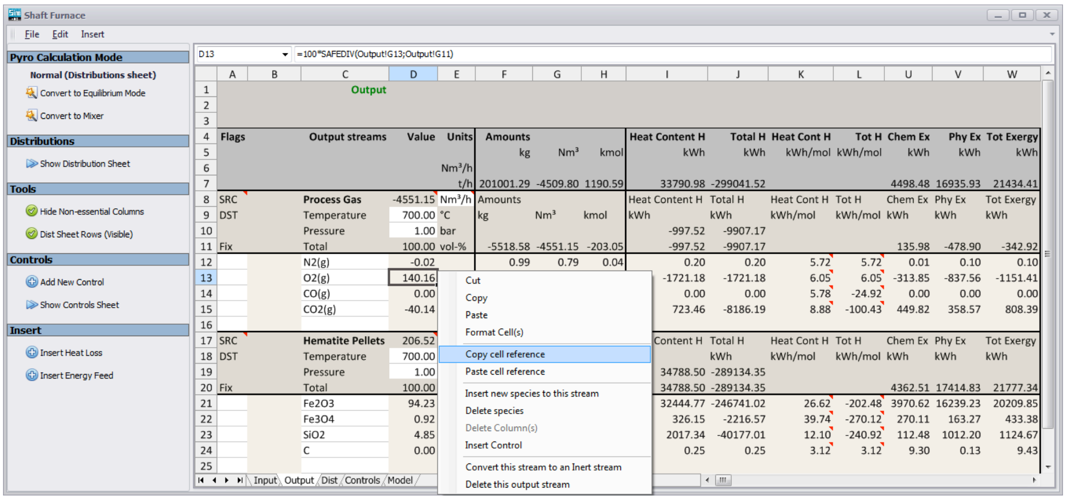

Fig. 21. Copy the cell reference of O2 % in the gas stream.

Then set this cell reference as the control by selecting Paste cell reference for the Measured value of the O2 % control, cell D12 (**Fig. 22**).

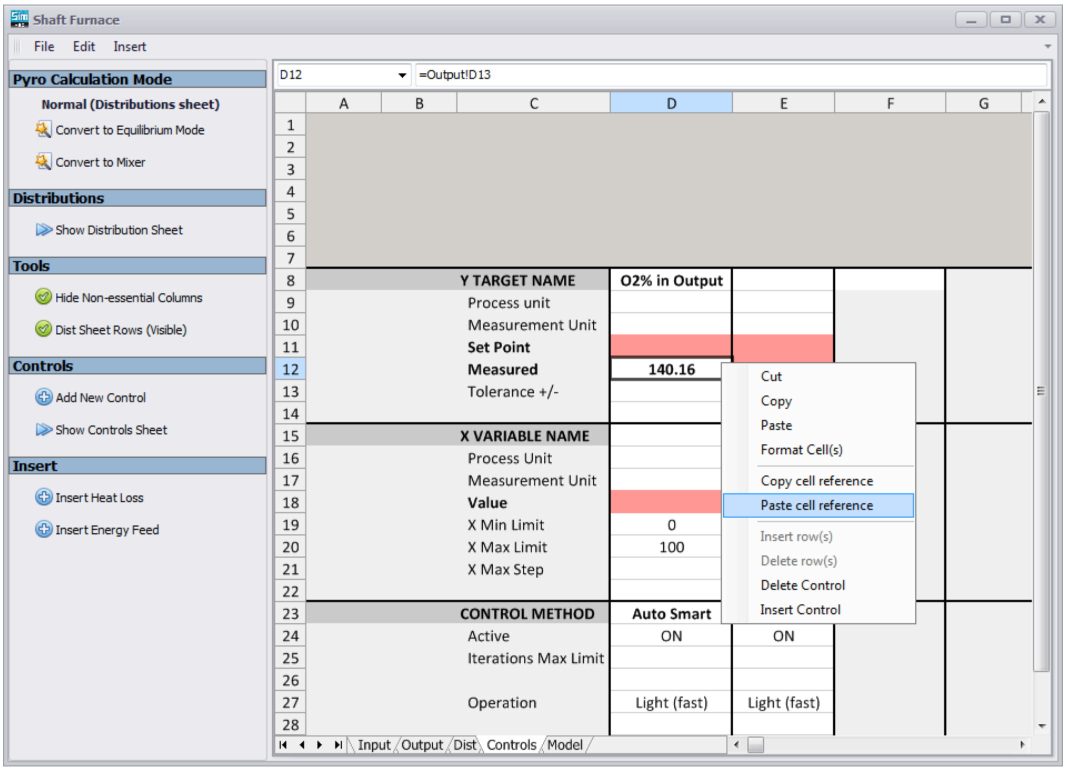

Fig. 22. Set cell reference for the target parameter.

For this target parameter you must assign the Set Point value, which will be the goal that the control tries to reach. In this example, the Set Point value will be 5.00 vol-%. It is also recommended to add the process unit and measurement unit to the control (**Fig. 23**). Having the units in the controls helps to keep track of their operation.

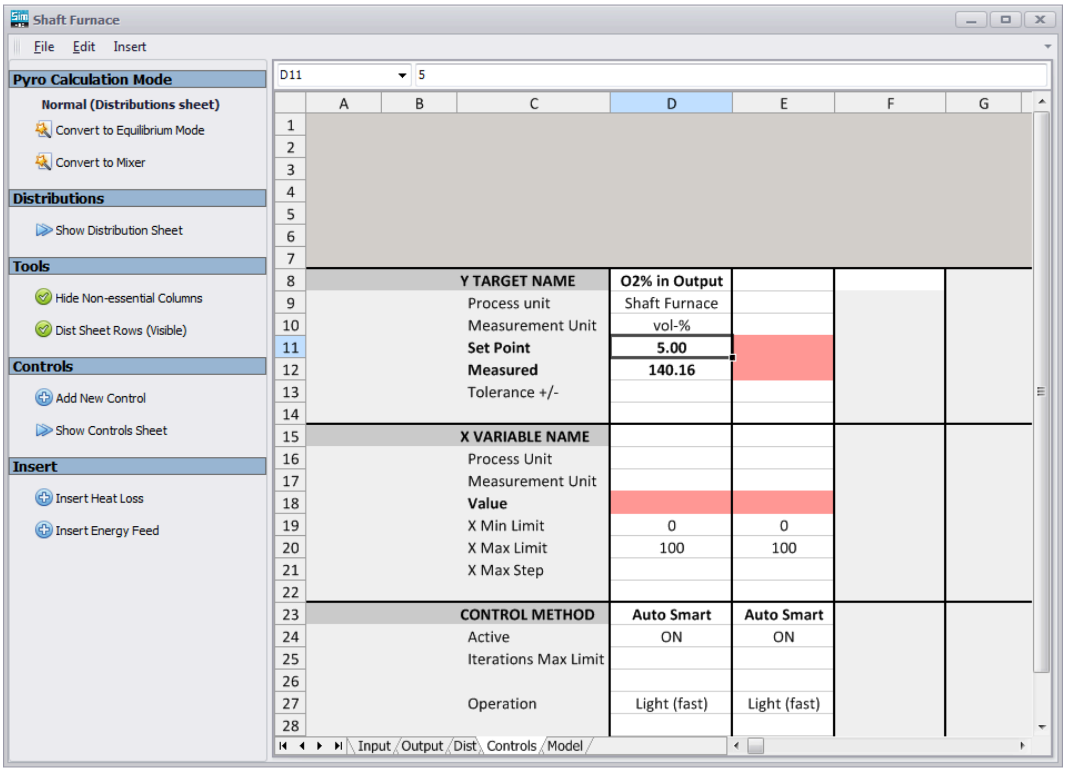

Fig. 23. Assign Set Point value for the control.

Next, set the variable cell reference that will regulate the target parameter. In this example, you can use the total input of the "Air" stream. To set this cell reference, go to the Input sheet and copy the correct cell reference (Input!D22) (**Fig. 24**), and paste the cell reference on the Controls sheet to the Value cell (Controls!D18). Also fill in the process and measurement unit information for the variable parameter (**Fig. 25**).

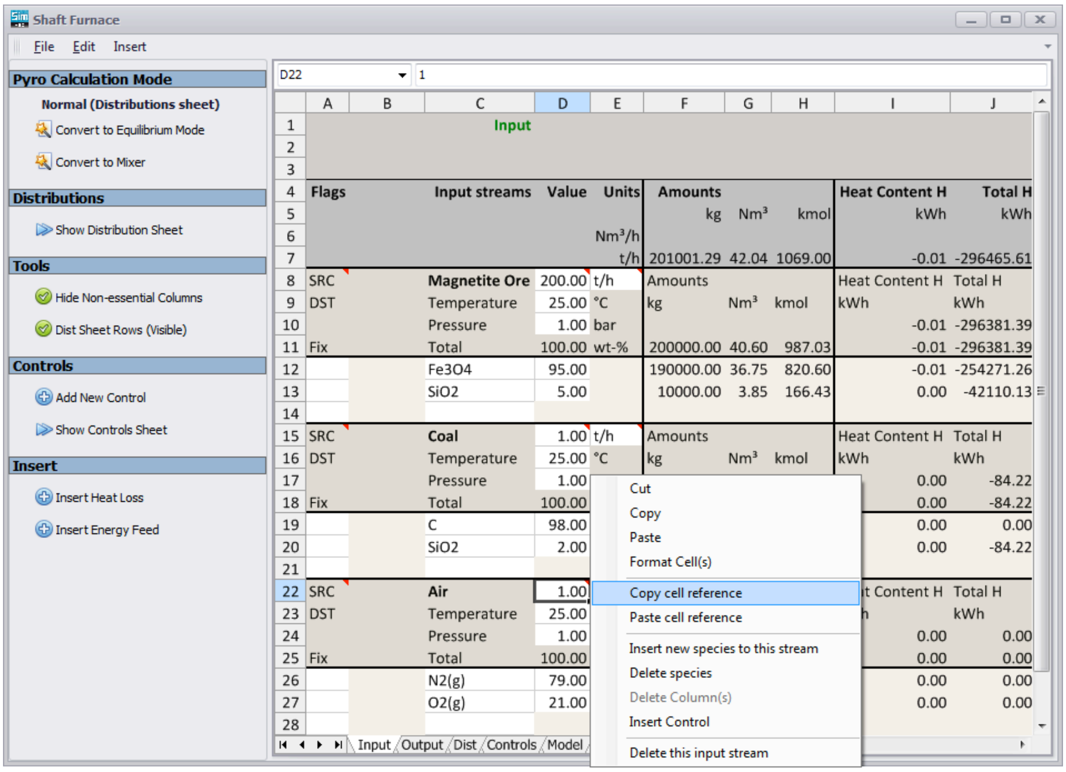

Fig. 24. Copy cell reference of the air feed.

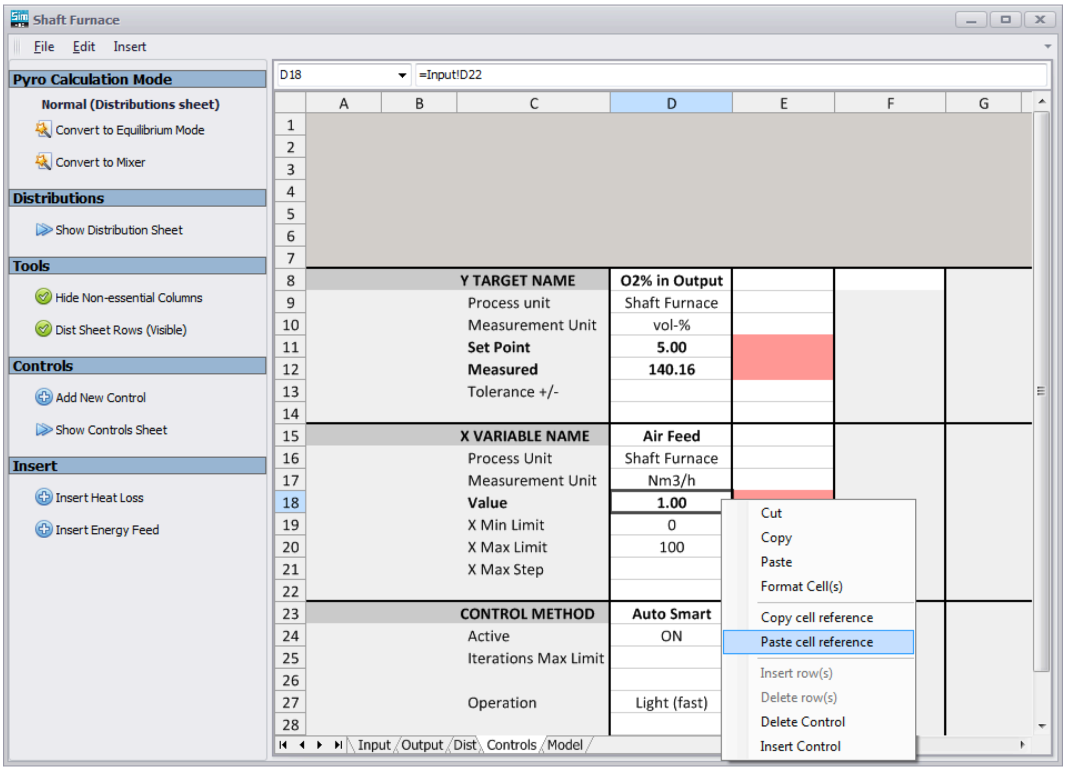

Fig. 25. Set cell reference for the variable parameter.

Finally, it is recommended to adjust the minimum and maximum limits for the variable parameter and to set a tolerance value for the target parameter (**Fig. 26**). After that the O2% control is ready.

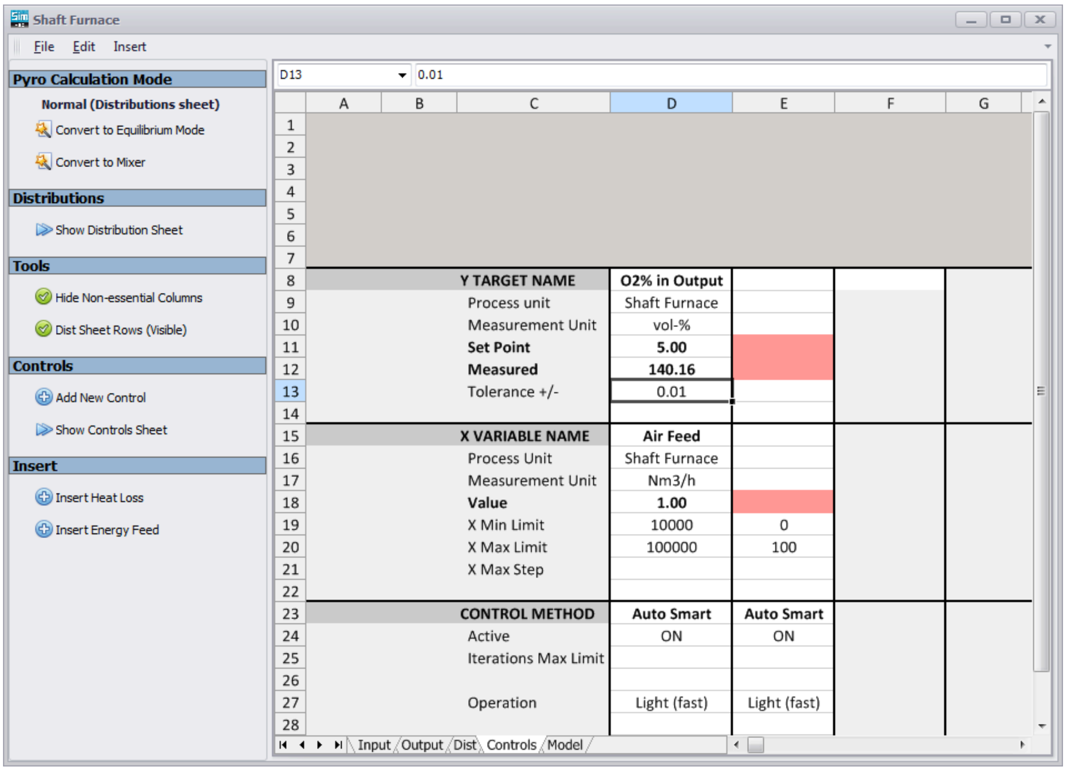

Fig. 26. Variable limits and target tolerance.

The Heat Balance control can be made by following the same steps. First, copy the cell reference for the Total H balance (Dist!J4) (**Fig. 27**).

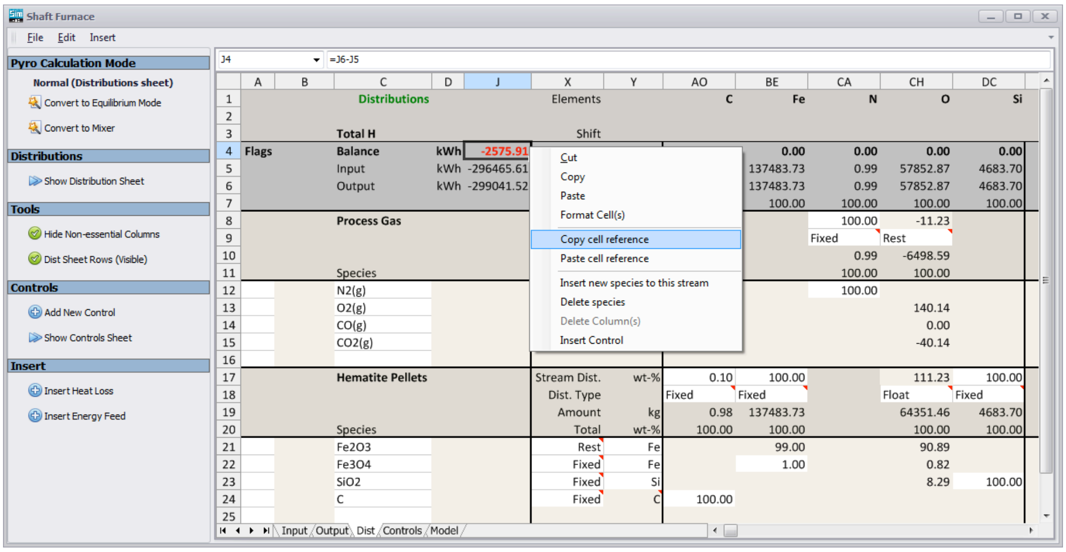

Fig. 27. Copy cell reference of the total enthalpy balance.

Then paste this cell reference to the Measured cell of the Heat Balance control and assign 0.00 as the Set Point (**Fig. 28**).

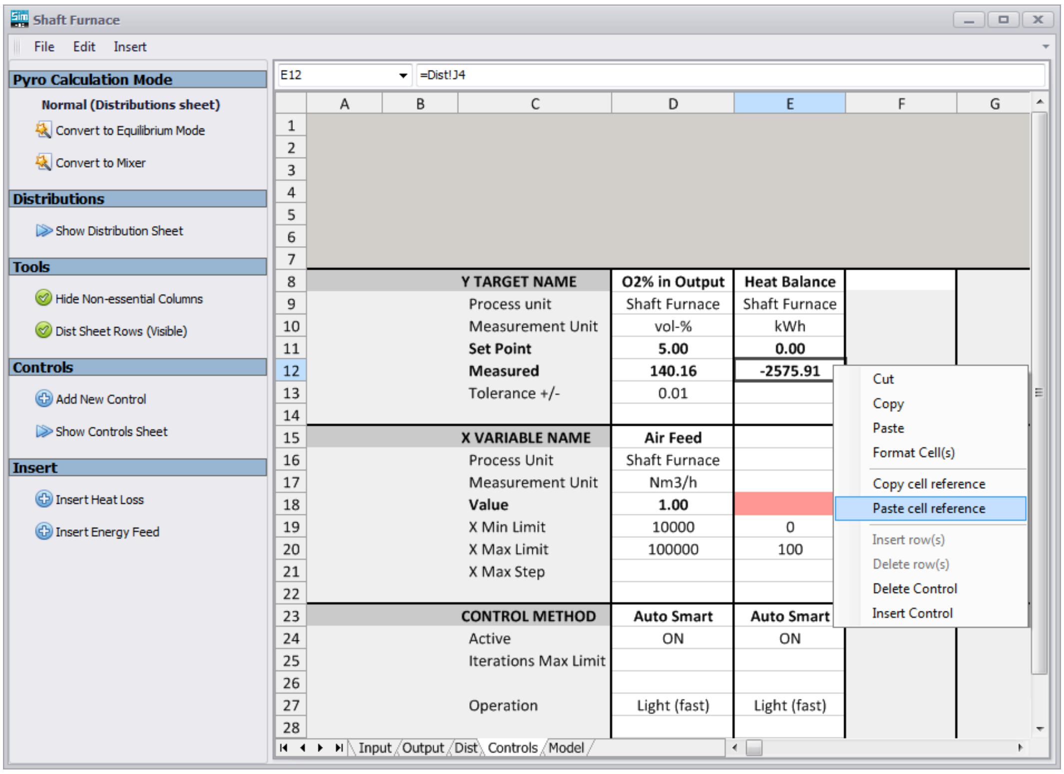

Fig. 28. Set the Total H balance as the target parameter.

The variable to regulate the heat balance can be set as the amount of coal fed into the furnace. Copy the cell reference of the "Coal" stream's total amount (Input!D15) (**Fig. 29**) and paste it to the Value cell of the Heat Balance control (**Fig. 30**).

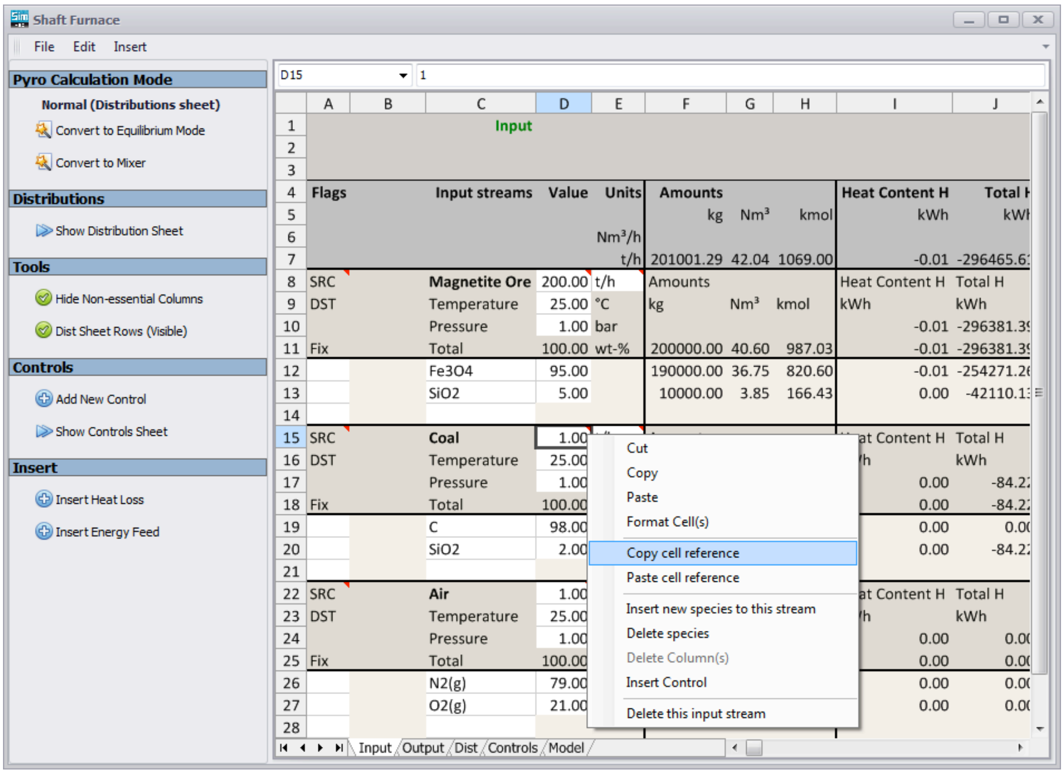

Fig. 29. Copy cell reference of the coal feed.

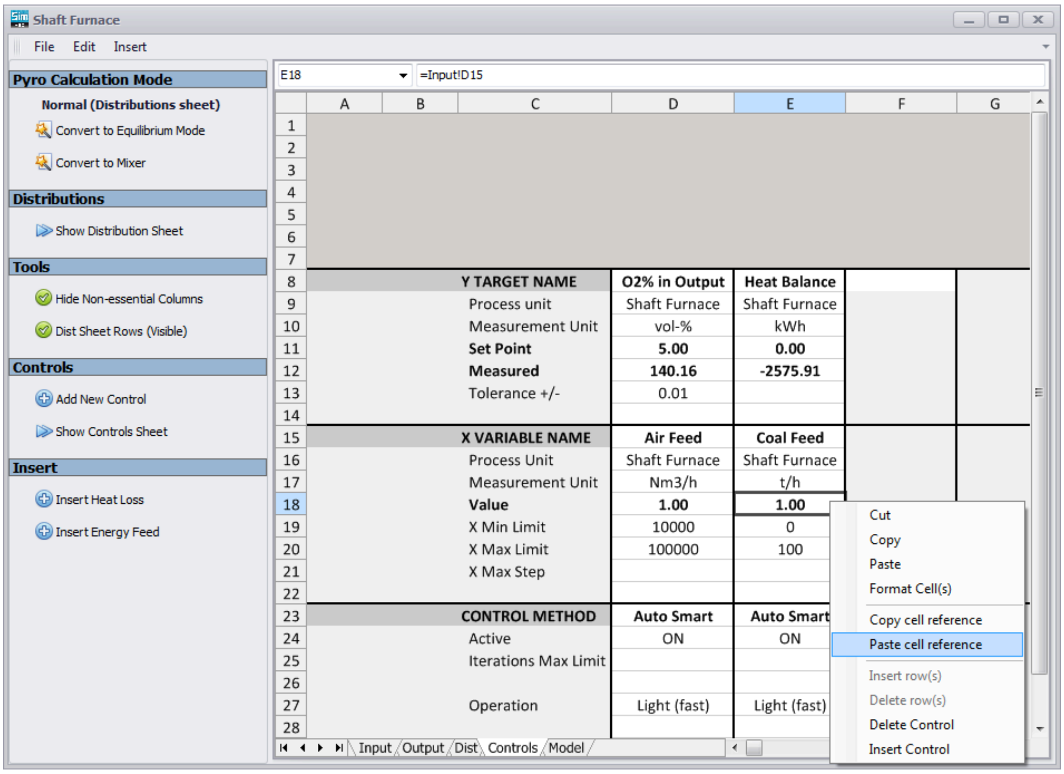

Fig. 30. Set Coal feed as the variable.

To complete the process controls, add a tolerance value for the heat balance and adjust the minimum and maximum limits for the coal feed (**Fig. 31**).

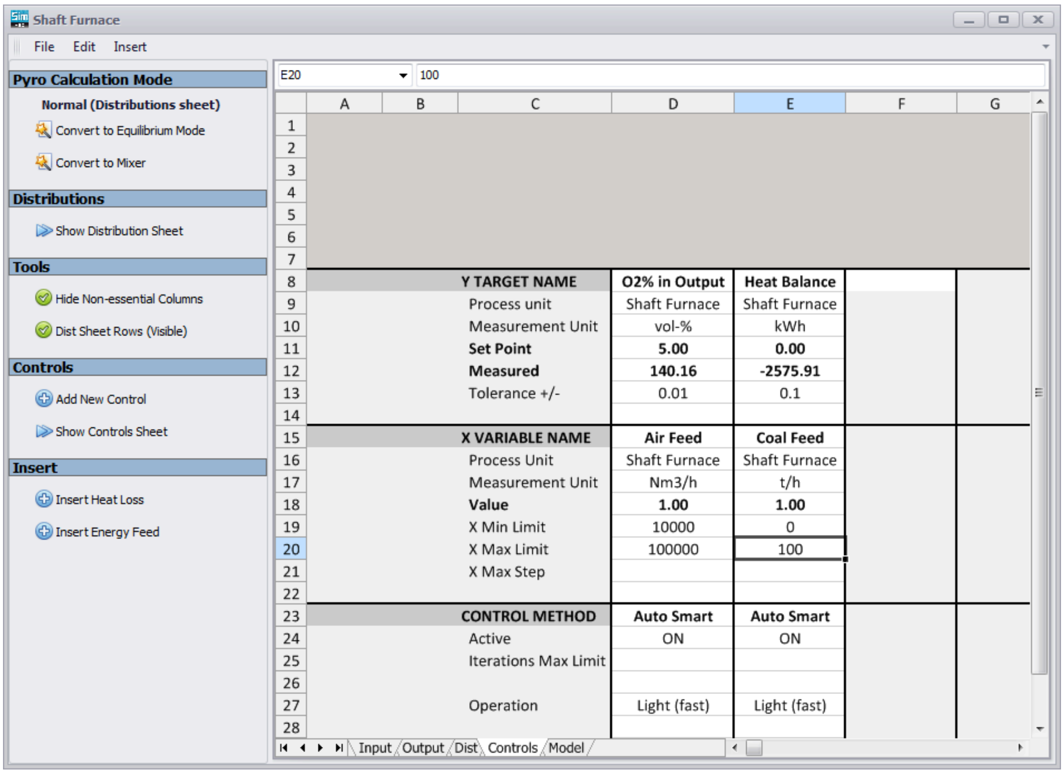

Fig. 31. Completed controls.

42.9. Step 9. Run the Process Model

The process model is now ready and you can start the simulation by pressing the Simulate button at the top bar (**Fig. 32**). Next to the Simulate button you can set the number of iteration rounds. Processes with recycling streams and controls may require several iteration rounds in order to reach steady state.

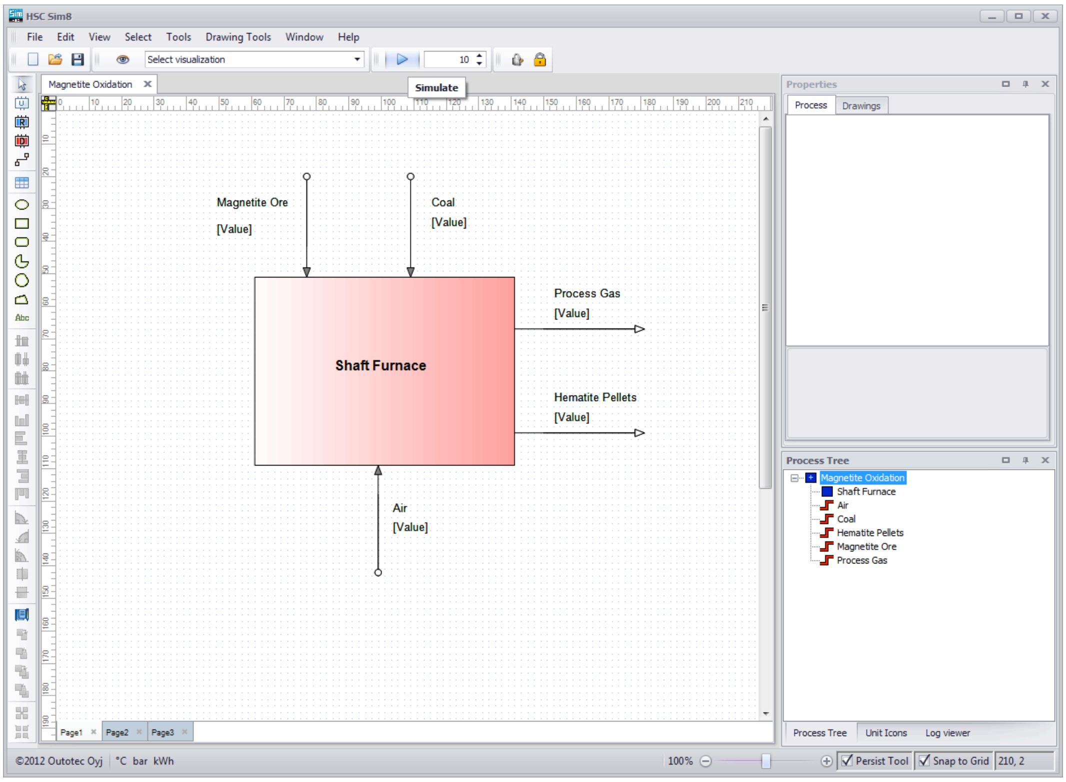

Fig. 32. Simulate the process.

Results of the simulation can be shown on the flowsheet by selecting the Stream Visualization Mode (**Fig. 33**). The selected property in the adjacent dropdown menu is shown in each of the stream value labels (**Fig. 34**).

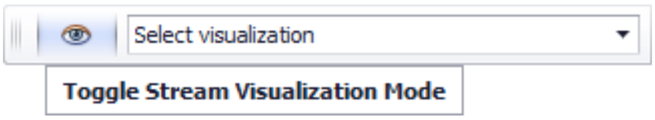

Fig. 33. Stream Visualization.

Visualization can be used with the simulation to study, whether the process reaches steady state. After a few simulation rounds, the value labels should obtain values which no longer change when further simulation rounds are run. It is also recommended to check the controls (**Fig. 35**). They are OK if the Set Point has been reached within the tolerance.

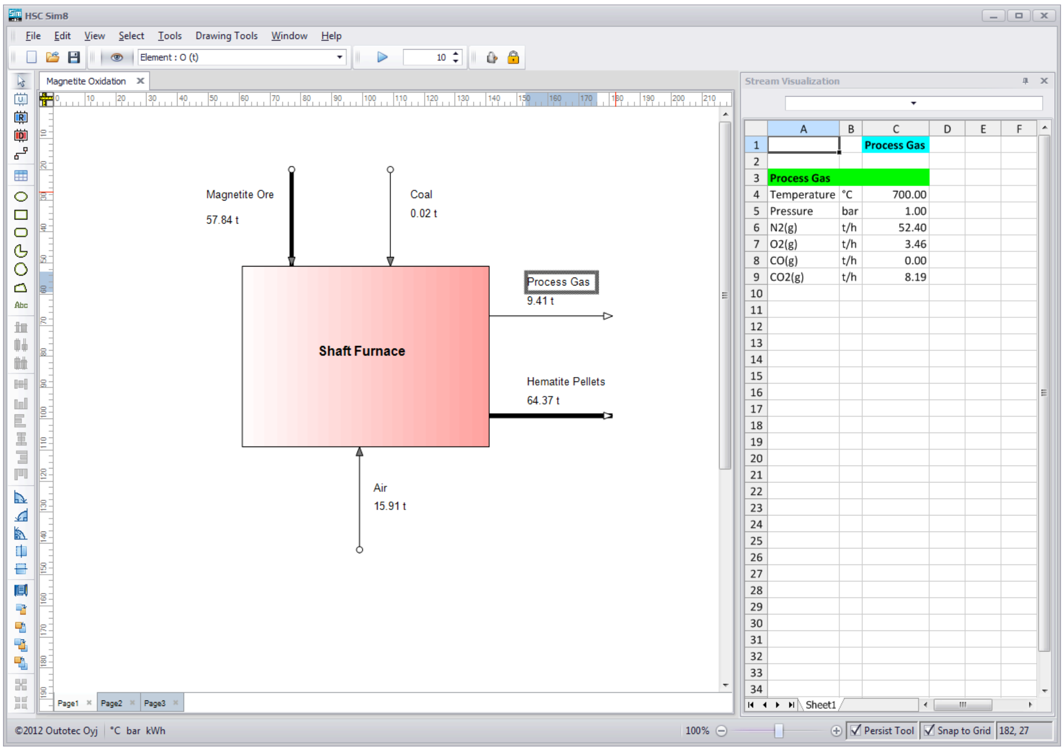

Fig. 34. Element balances and behavior can be seen when element amounts are selected in the visualization. In this screenshot, the diagram shows the behavior of oxygen in the process.

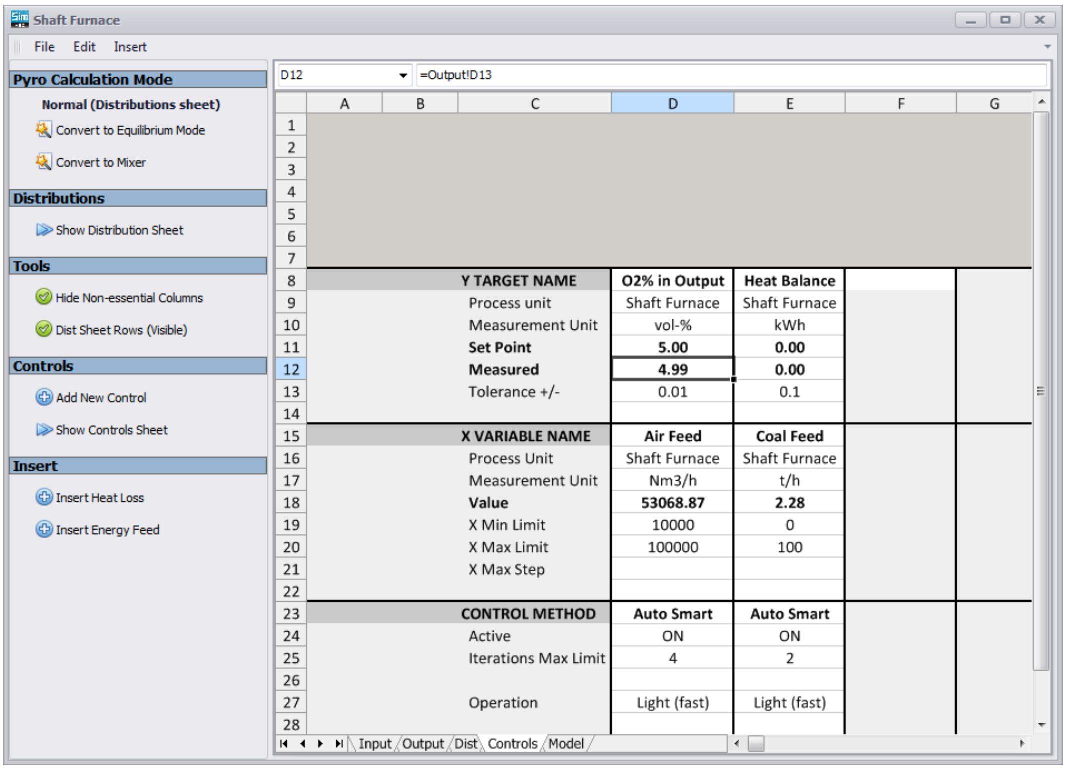

Fig. 35. Controls after simulation.