44. Sim Reactions Example

44.1. General

This example contains instructions on how to create a simple leaching reactor model where 10 t/h of FeS is leached with acid (H_2SO_4) and air at 70 °C. The water feed is 50 t/h and the FeS leaching efficiency is 90 %, oxygen efficiency is 50 %, and the acid concentration in the product is 1 g/l.

The reactor is cooled with cooling coils. The cooling water input temperature is 25 °C and output temperature 60 °C.

You should keep in mind that streams are put into the input and output sheets in the same order as you have drawn them. This means that when you make a new model the streams might be in a different column than explained here.

The example files can be found from the HSC Chemistry installation folder …Flowsheet_Hydro\Hydro_example3\Hydro_example3.Sim8. This example describes the creation of the flowsheet in detail with references to the Sim Flowsheet manual.

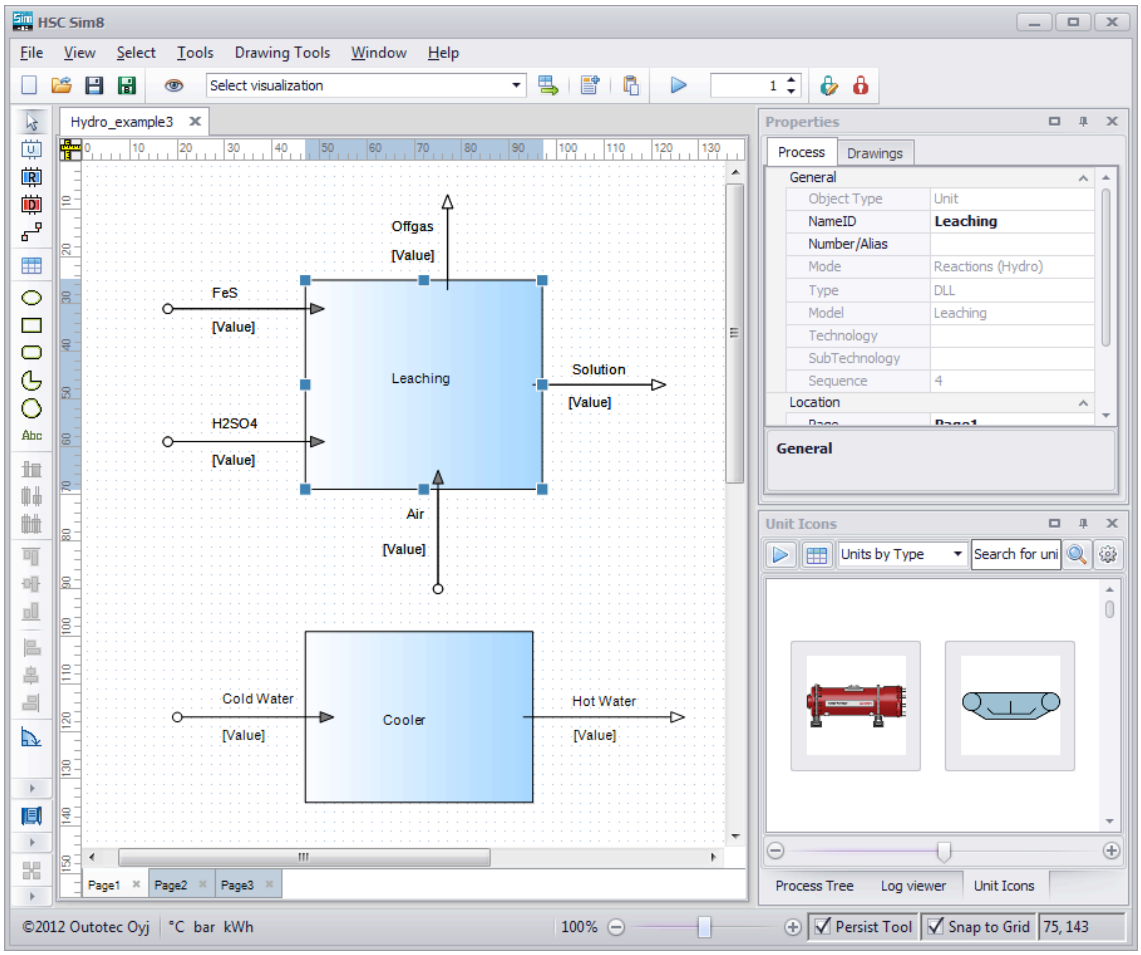


Fig. 1. Sim Reactions Example flowsheet.

44.2. Steps to Successful Sim Reactions Simulation

1. Draw units and streams
2. Save process and save backup
3. Create variable list
4. Add reaction equations
5. Specify distributions
6. Set controls
7. Specify raw material amounts
8. Save process
9. Run process

44.2.1. Drawing a Flowsheet, See Chapter 40 (section 40.1.)

- Draw Reactions **units** (blue).
- Draw input and output **streams**. Left mouse click to start and make corners and double-click to end the stream. For editing the stream afterwards, see section 40.1.2.
- Name the units and streams, see **Fig. 1** and Chapter 40 (section 40.1.3.).
- Check that the source and destination for the streams are correct.

44.2.2. Setting the Variable List, See Chapter 43 (section 43.2.)

A) Import Ready-Made Variable List

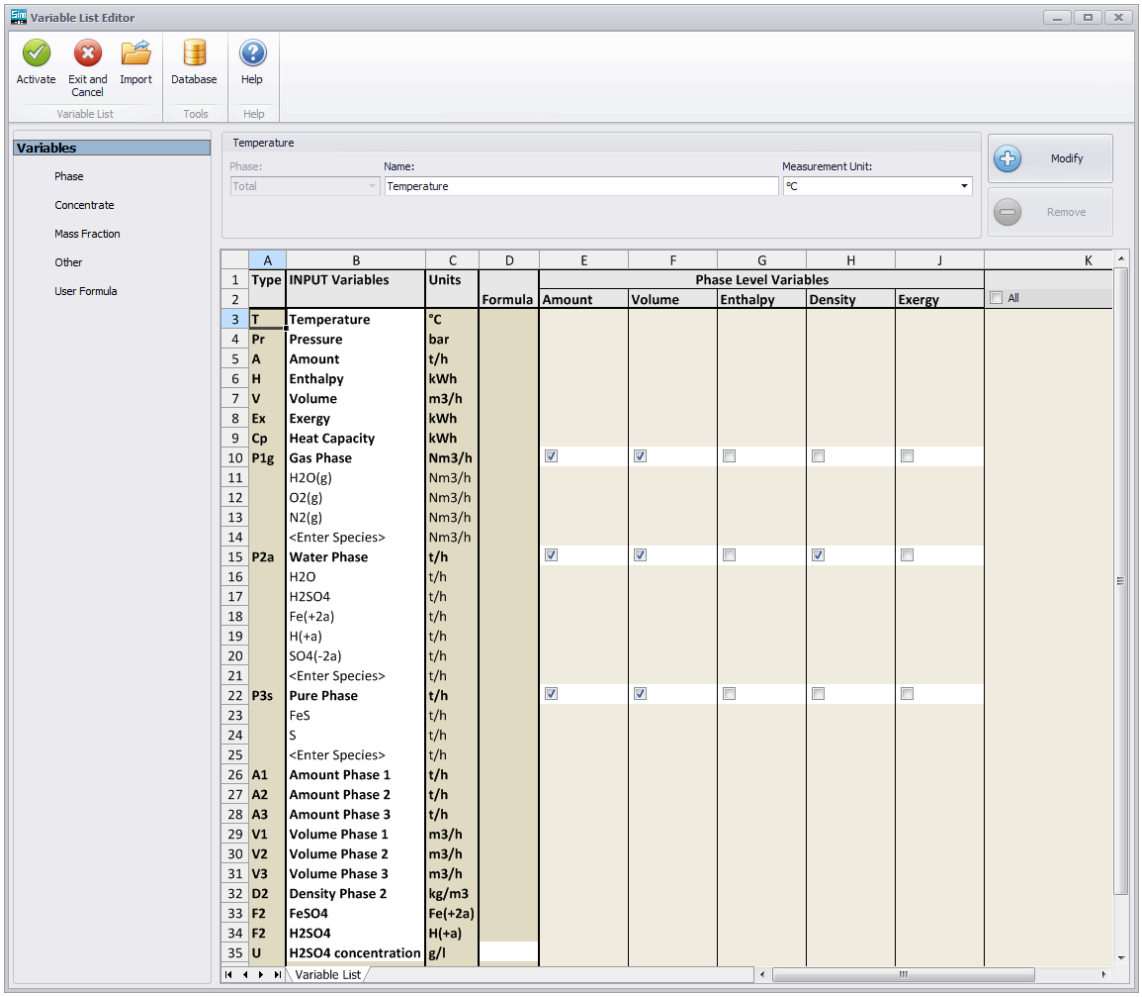
In this example two **variable lists** can be used. You can add the lists to the model by double-clicking the unit and clicking Variable List Editor (or in Excel editor, Tools menu and Variable List Editor) and by pressing Import…\Flowsheet_Hydro\Hydro_example3\. For the **Leaching unit** we choose Leaching.xlsx and for the **Cooler unit** Cooler.xlsx, see **Fig. 2** and **Fig. 3**. It is also possible to use Leaching.xlsx list for the Cooler unit but not vice versa.

B) Fill Variable List Manually

You can also fill in the variable lists manually, see **Fig. 2** and **Fig. 3,** or Chapter 43. Use Nm3/h unit for the Gas Phase. You need to give the mass fractions of the water phase otherwise density cannot be calculated (see rows 33-34 in **Fig. 2**). Since H_2SO_4 concentration in g/l is not in the list, you need to create a User Formula (U) in the Variable List Editor.

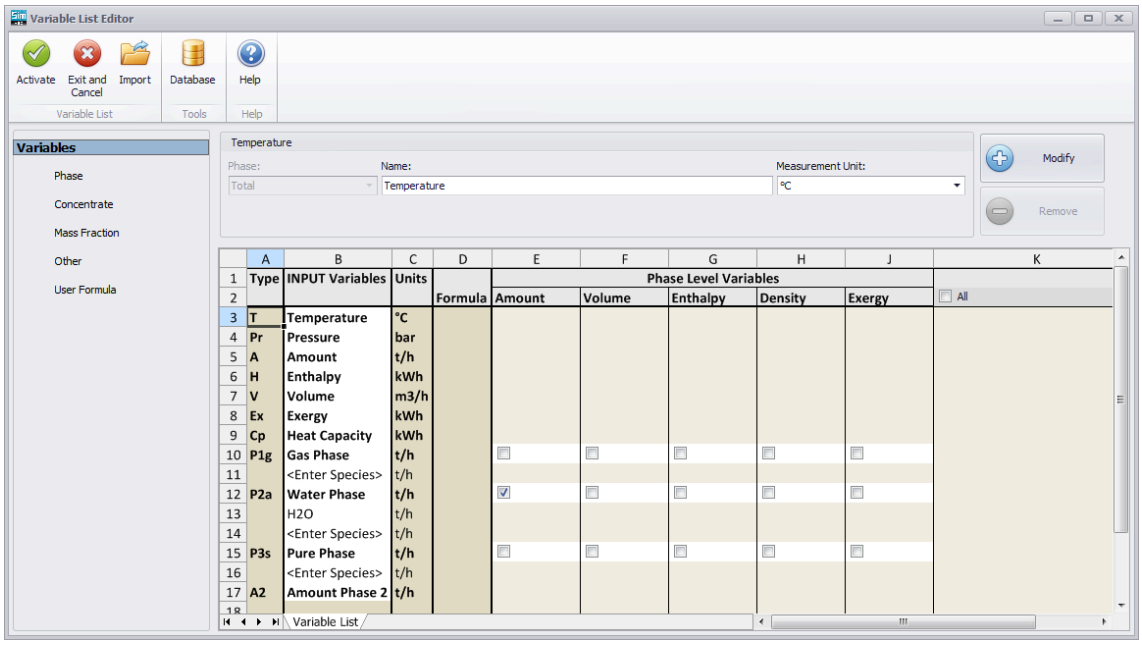
- Choose User formula and give it a name (H_2SO_4 concentration) and measure unit (g/l).
- Make the formula in column D, see **Fig. 2**. In the example above, the formula in cell D35 is D19/MW(“H”)/2*MW(“H2SO4”)/D30*1000, which means that mass of H_2SO_4 is calculated from the amount of H(+a) ions in moles (see equation in **Fig. 4**) divided by the water phase volume. The result is multiplied by 1000 to obtain the unit grams of H_2SO_4 per liter of solution.
- The User formula is copied automatically to all the Input and Output streams of each unit when Activate is clicked. NB! The equation is changed in the Variable List Editor to “=SAFEDIV(SAFEDIV(D19;MW("H"))/2*MW("H2SO4");D30)*1000” (with equation SAFEDIV HSC8 Sim sets 0/0 = 0).

When modifying the variable list, remember that columns A to D are automatically synchronized, which means that any changes are automatically copied to all the streams.



	A	B	C	D	E	F	G	H	J	K
1	Type	INPUT Variables	Units		Phase Level Variables					
2				Formula	Amount	Volume	Enthalpy	Density	Exergy	All
3	T	Temperature	°C							
4	Pr	Pressure	bar							
5	A	Amount	t/h							
6	H	Enthalpy	kWh							
7	V	Volume	m3/h							
8	Ex	Exergy	kWh							
9	Cp	Heat Capacity	kWh							
10	P1g	Gas Phase	Nm3/h		☑	☑	☐	☐	☐	
11		H2O(g)	Nm3/h							
12		O2(g)	Nm3/h							
13		N2(g)	Nm3/h							
14		<Enter Species>	Nm3/h							
15	P2a	Water Phase	t/h		☑	☑	☐	☑	☐	
16		H2O	t/h							
17		H2SO4	t/h							
18		Fe(+2a)	t/h							
19		H(+a)	t/h							
20		SO4(-2a)	t/h							
21		<Enter Species>	t/h							
22	P3s	Pure Phase	t/h		☑	☑	☐	☐	☐	
23		FeS	t/h							
24		S	t/h							
25		<Enter Species>	t/h							
26	A1	Amount Phase 1	t/h							
27	A2	Amount Phase 2	t/h							
28	A3	Amount Phase 3	t/h							
29	V1	Volume Phase 1	m3/h							
30	V2	Volume Phase 2	m3/h							
31	V3	Volume Phase 3	m3/h							
32	D2	Density Phase 2	kg/m3							
33	F2	FeSO4	Fe(+2a)							
34	F2	H2SO4	H(+a)							
35	U	H2SO4 concentration	g/l							

Fig. 2. Variable list of the Leaching unit.



	A	B	C	D	E	F	G	H	J	K
1	Type	INPUT Variables	Units		Phase Level Variables					
2				Formula	Amount	Volume	Enthalpy	Density	Exergy	All
3	T	Temperature	°C							
4	Pr	Pressure	bar							
5	A	Amount	t/h							
6	H	Enthalpy	kWh							
7	V	Volume	m3/h							
8	Ex	Exergy	kWh							
9	Cp	Heat Capacity	kWh							
10	P1g	Gas Phase	t/h		☐	☐	☐	☐	☐	
11		<Enter Species>	t/h							
12	P2a	Water Phase	t/h		☑	☐	☐	☐	☐	
13		H2O	t/h							
14		<Enter Species>	t/h							
15	P3s	Pure Phase	t/h		☐	☐	☐	☐	☐	
16		<Enter Species>	t/h							
17	A2	Amount Phase 2	t/h							

Fig. 3. Variable list of the Cooler unit.

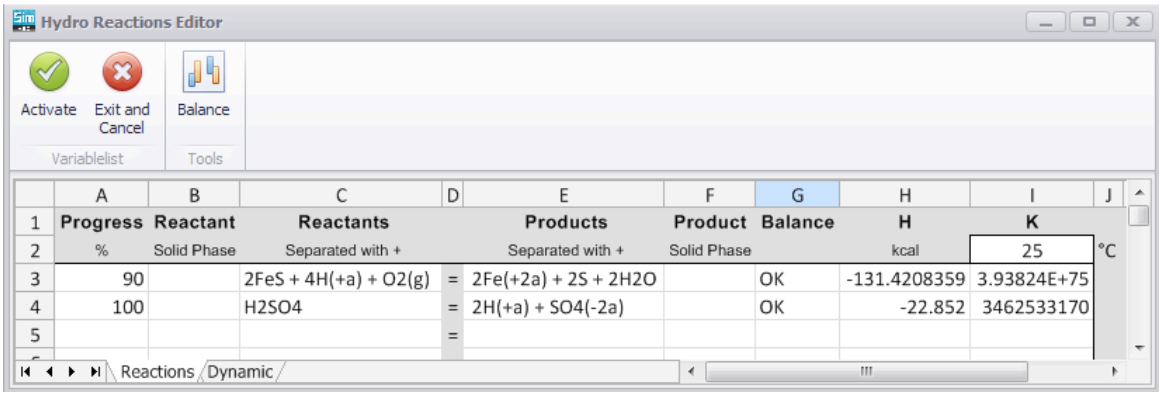
44.2.3. Add Reaction Equations to the Unit (Chapter 43 section 43.3.)

The following leaching reaction equations:

$FeS + H(+a) + O_2(g) = Fe(+2a) + S + H_2O$ (90 % efficiency)

$H_2SO_4 = H(+a) + SO_4(-2a)$ (100 % efficiency)

can be added with the Chemical Reactions Wizard. In the **Leaching unit**, open the Excel editor "Chemical Reactions Wizard". You have to write the Progress %, Reactants, Products, and press the Balance button, which checks the coefficients for the reactions, see **Fig. 4**.

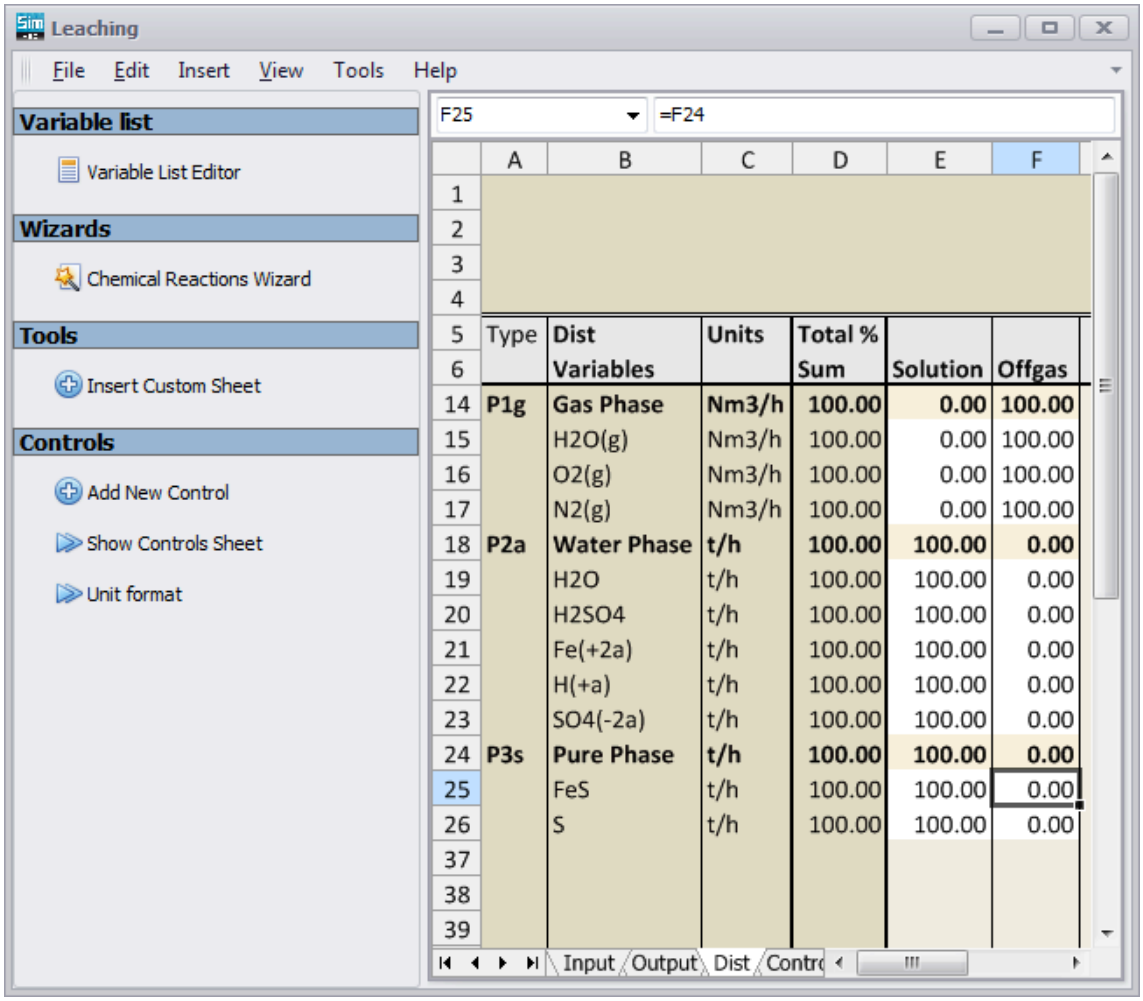


	A	B	C	D	E	F	G	H	I	J
1	Progress	Reactant	Reactants		Products	Product	Balance	H	K	
2	%	Solid Phase	Separated with +		Separated with +	Solid Phase		kcal	25	°C
3	90		2FeS + 4H(+a) + O2(g)	=	2Fe(+2a) + 2S + 2H2O		OK	-131.4208359	3.93824E+75	
4	100		H2SO4	=	2H(+a) + SO4(-2a)		OK	-22.852	3462533170	
5				=						

Fig. 4. Reactions sheet in Chemical Reactions Wizard.

44.2.4. Specify Distributions

Remember to complete the **Dist** sheets of the units. In the Leaching unit, 100% of the gas phase goes to the Offgas stream and 100% of the liquid and solid phase goes to the Solution stream. Fill in the percentages for both streams, see **Fig. 5**. In the **Cooler unit** there is just one output stream so fill in 100 % to each phase.



	A	B	C	D	E	F
1						
2						
3						
4						
5	Type	Dist	Units	Total %		
6		Variables		Sum	Solution	Offgas
14	**P1g**	**Gas Phase**	**Nm3/h**	**100.00**	**0.00**	**100.00**
15		H2O(g)	Nm3/h	100.00	0.00	100.00
16		O2(g)	Nm3/h	100.00	0.00	100.00
17		N2(g)	Nm3/h	100.00	0.00	100.00
18	**P2a**	**Water Phase**	**t/h**	**100.00**	**100.00**	**0.00**
19		H2O	t/h	100.00	100.00	0.00
20		H2SO4	t/h	100.00	100.00	0.00
21		Fe(+2a)	t/h	100.00	100.00	0.00
22		H(+a)	t/h	100.00	100.00	0.00
23		SO4(-2a)	t/h	100.00	100.00	0.00
24	**P3s**	**Pure Phase**	**t/h**	**100.00**	**100.00**	**0.00**
25		FeS	t/h	100.00	100.00	0.00
26		S	t/h	100.00	100.00	0.00
37						
38						
39						

Fig. 5. Dist. sheet of the Leaching unit.

44.2.5. Setting Controls for the Process, Chapter 43 (section 43.5.)

Controls can be added, removed and seen using quick links on the left column, see **Fig. 6**.

In the first control sheet, the H_2SO_4 concentration after leaching is set at 1 g/l of solution by calculating the input amount of H_2SO_4, see **Fig. 6** and **Table 1**.

In the second control sheet, the cooling requirements (heat balance) of the highly exothermic leaching process are set to 0 by calculating the cooling water amount. NB! Insert an extra sheet in the Cooler unit, see **Fig. 7** to **Fig. 10** and **Table 2**.

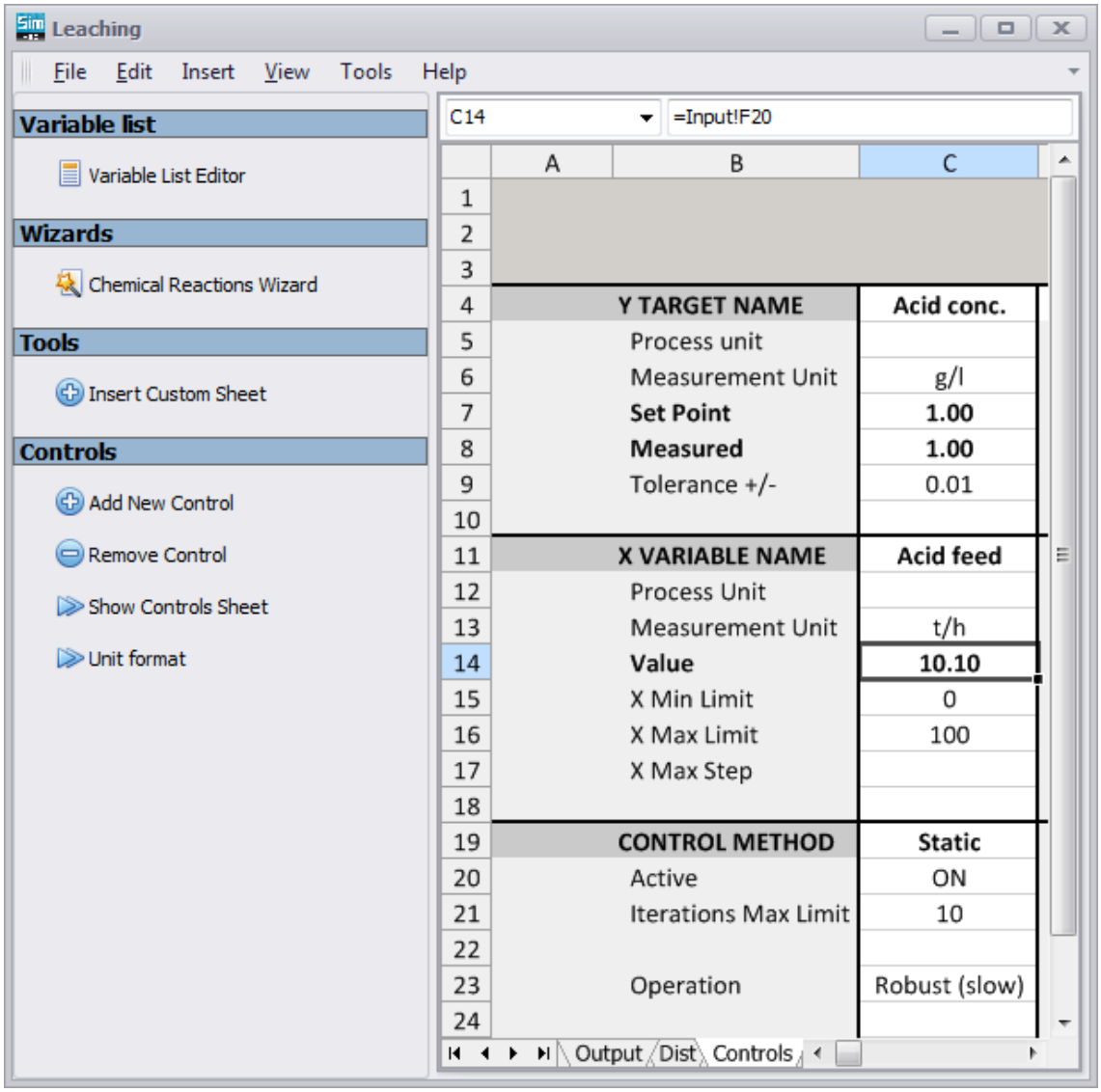


Fig. 6. Controls sheet of the Leaching unit.

Table 1. Data for controlling the H_2SO_4 concentration after leaching.

Row name (Cell)	Filled value or formula	Notes
Set point (C7)	1	Desired H_2SO_4 concentration, g/l
Measured (C8)	=Output!E36	Measured H_2SO_4 concentration, g/l
Tolerance +/- (C9)	0.01	Tolerance for concentration
Value (C14)	=Input!F20	H_2SO_4 input to the process, t/h
X Min Limit (C15)	0	Minimum amount for H_2SO_4 input
X Max Limit (C16)	100	Maximum amount for H_2SO_4 input

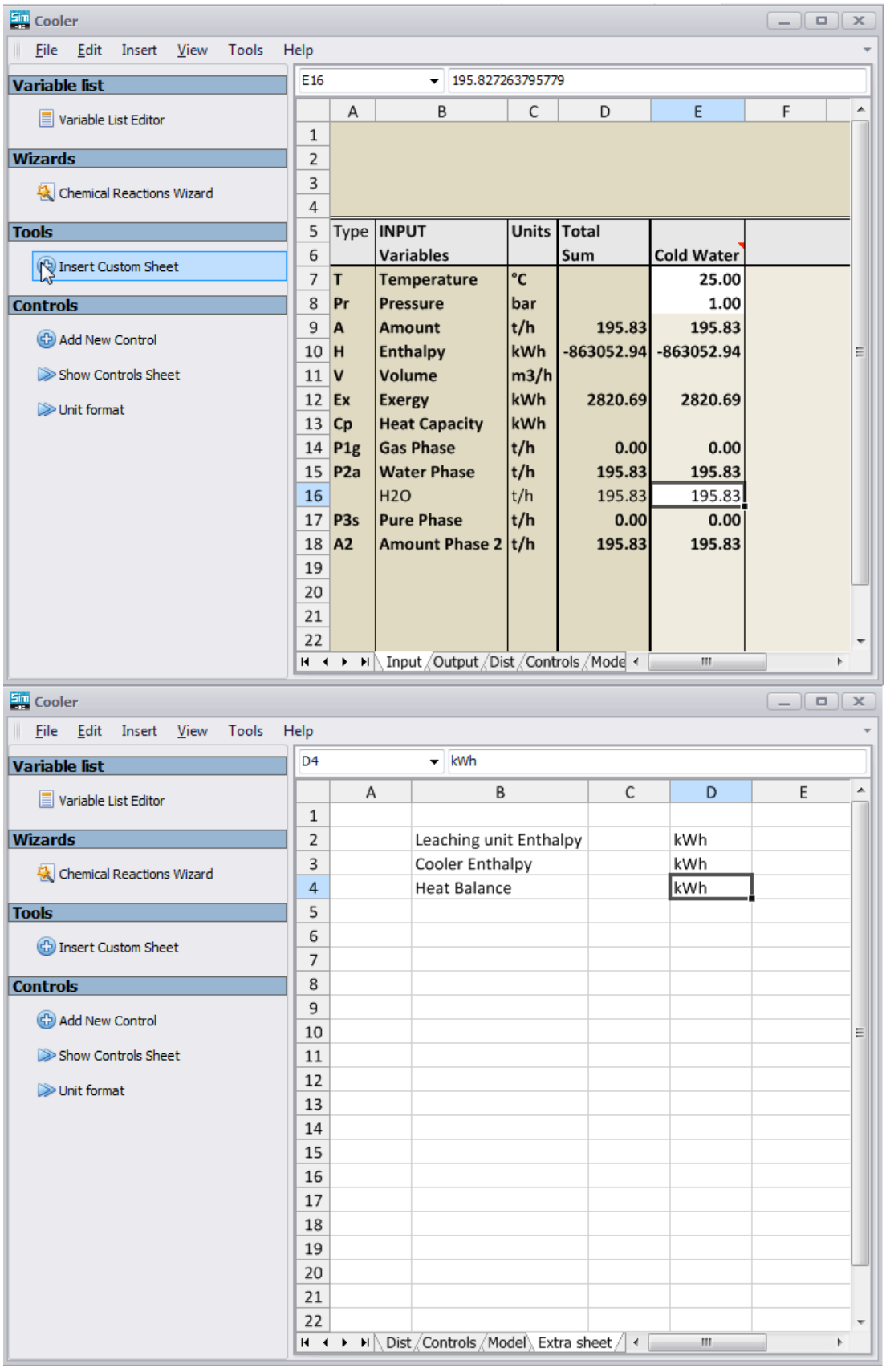


Fig. 7. Insert Custom Sheet and text added to this new sheet (renamed to Extra sheet).

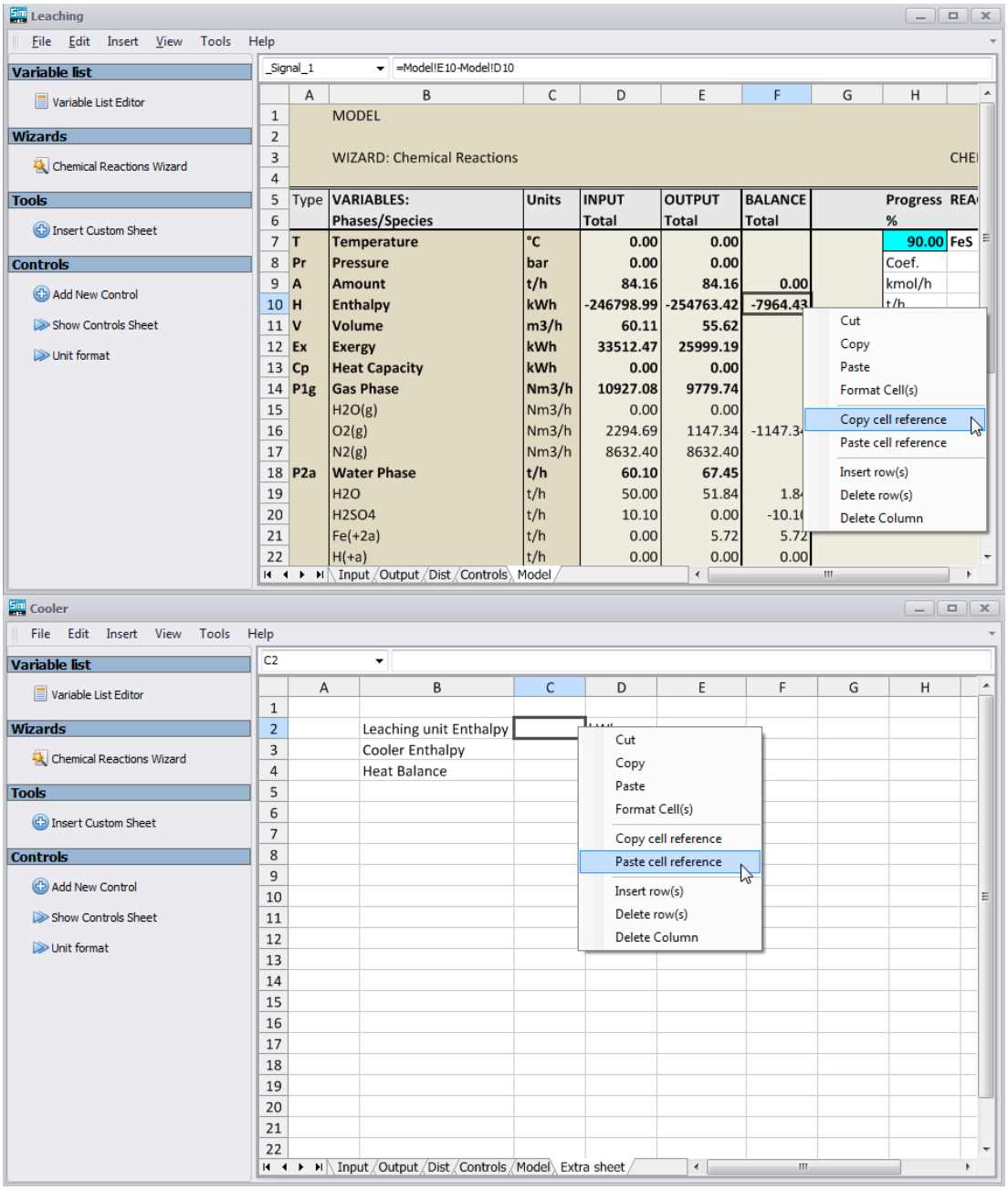


Fig. 8. Copy cell reference from the Leaching unit and paste cell reference to the extra sheet.

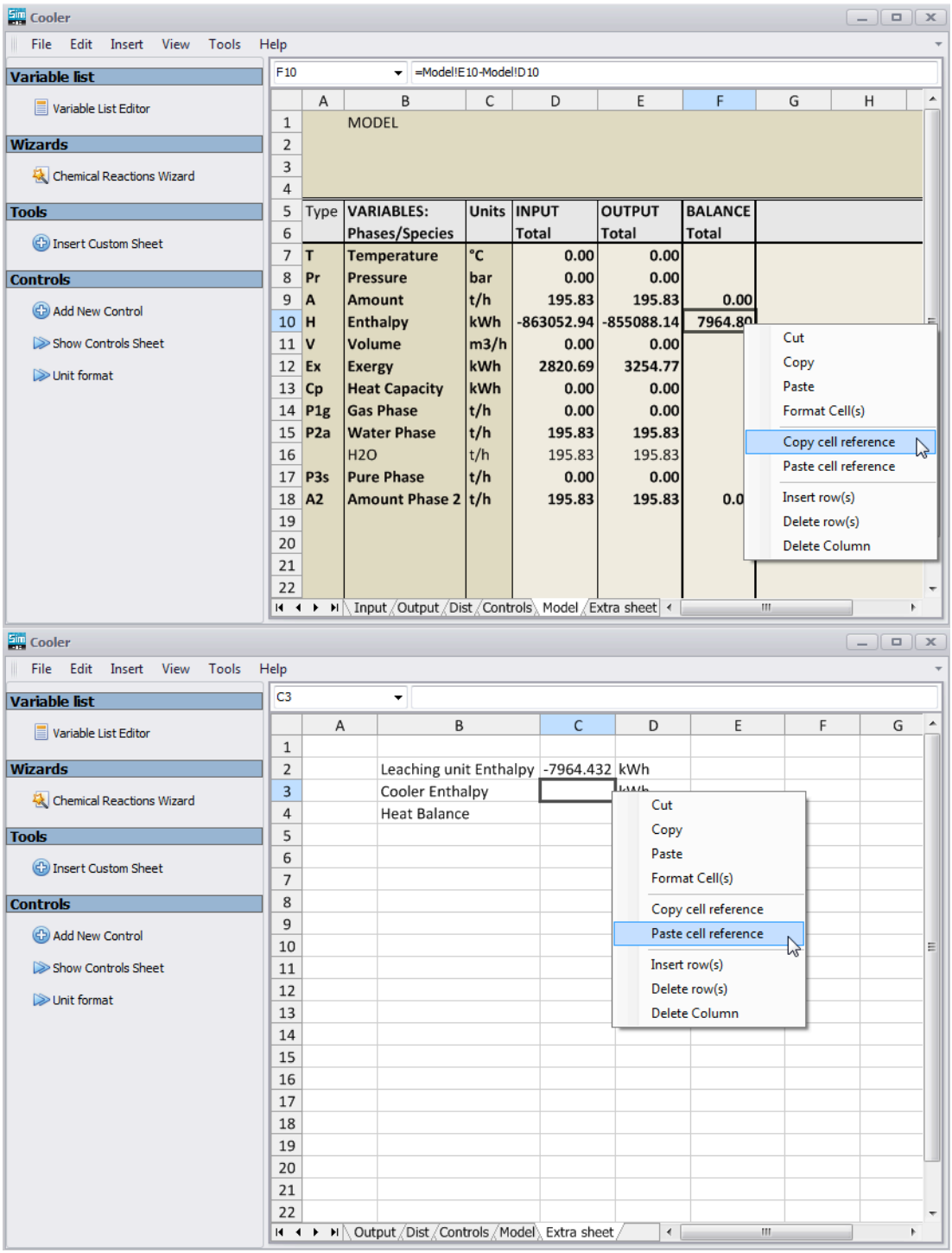


Fig. 9. Copy cell reference from the Cooler unit and paste cell reference to the extra sheet.

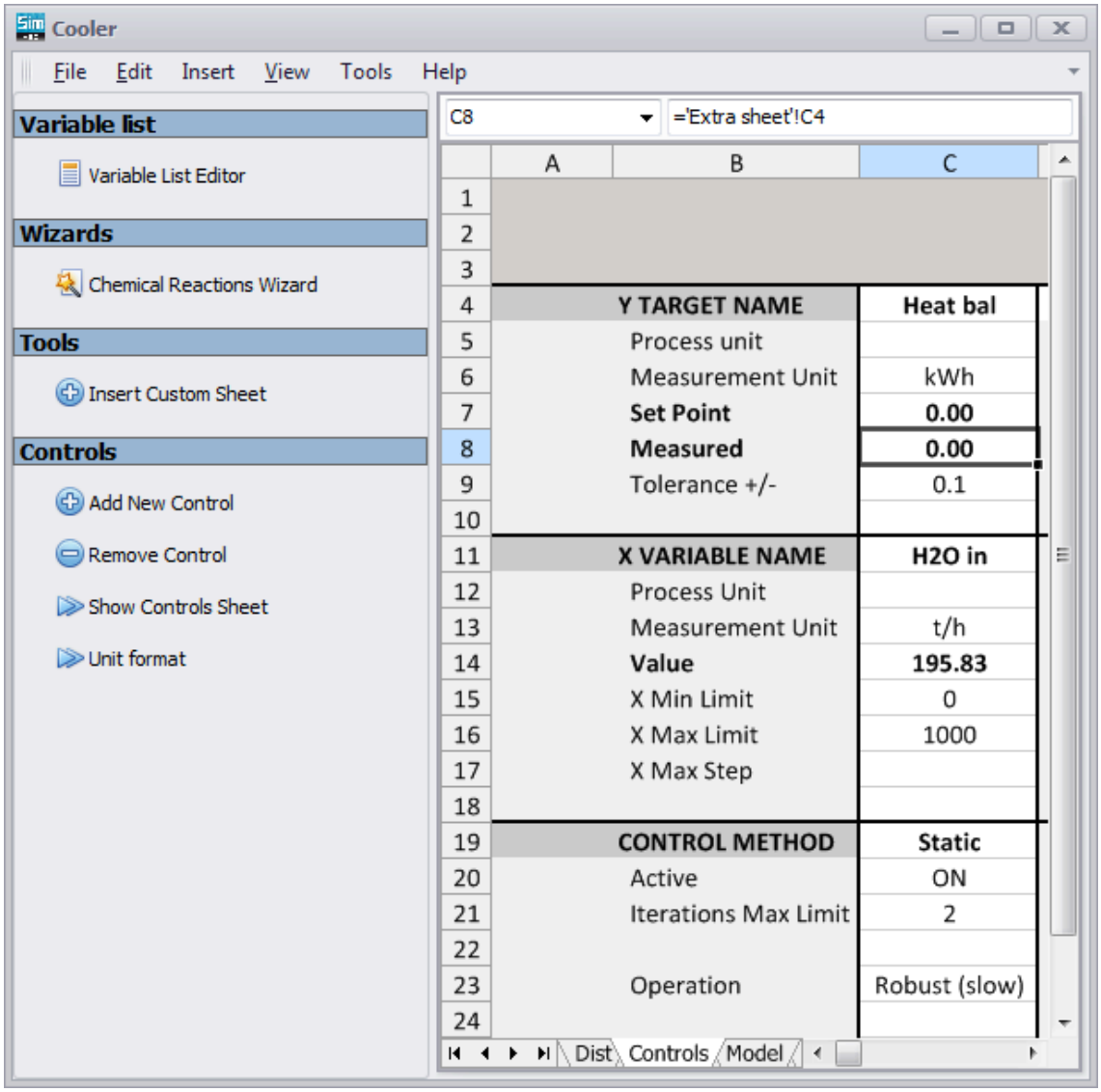


Fig. 10. Controls sheet of the Cooler unit.

Table 2. Data for controlling the Heat balance. Measured value is calculated in an additional sheet.

Row name (Cell)	Filled value or formula	Notes
Set point (C7)	0	Desired Heat balance, kWh
Measured (C8)	=Extra sheet!C4	Measured Heat balance, kWh
Tolerance +/- (C9)	0.1	Tolerance for Heat balance
Value (C14)	=Input!E16	H_2O input to the process, t/h
X Min Limit (C15)	0	Minimum amount for H_2O input
X Max Limit (C16)	1000	Maximum amount for H_2O input

44.2.6. Setting Feed Streams to the Process

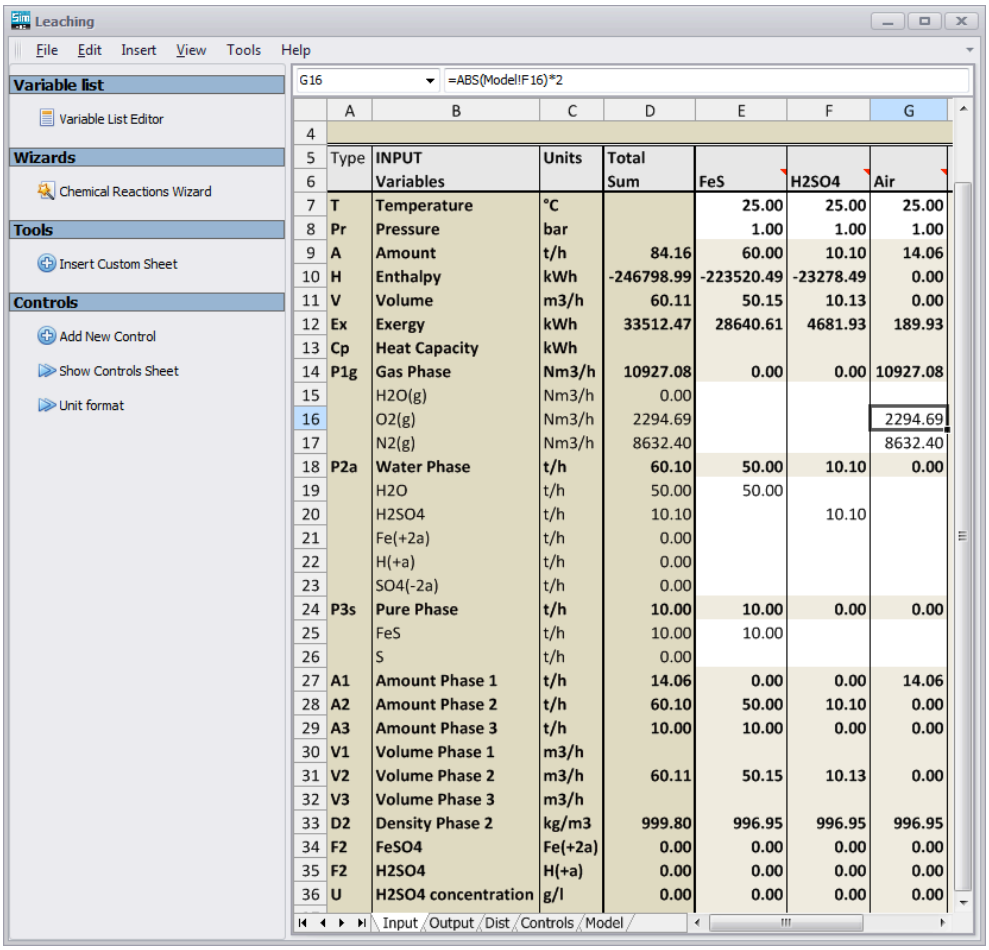
All the **feed streams** to the process should be set. If the feed to the process is not set, the stream will be ignored.

Input sheets of both Leaching and Cooler units:

- FeS stream H_2O is 50 t/h and FeS is 10 t/h in the FeS stream.
- H_2SO_4 stream sulfuric acid feed - an initial guess of 1 t/h can be given. Real value (10.1 t/h) is calculated using the control, see **Table 1**.
- Air stream consists of 21 vol.% of O_2(g) and 79 vol.% of N_2(g). Oxygen efficiency is 50 %, which means that 2 times the stoichiometric amount is needed. The formulas made for oxygen and nitrogen are =ABS(Model!F16)*2 and =G16/21*79, respectively.
- Cold water stream feed - an initial guess of 10 t/h can be given. Real value (195.8 t/h) is calculated using the control, see **Table 2**.

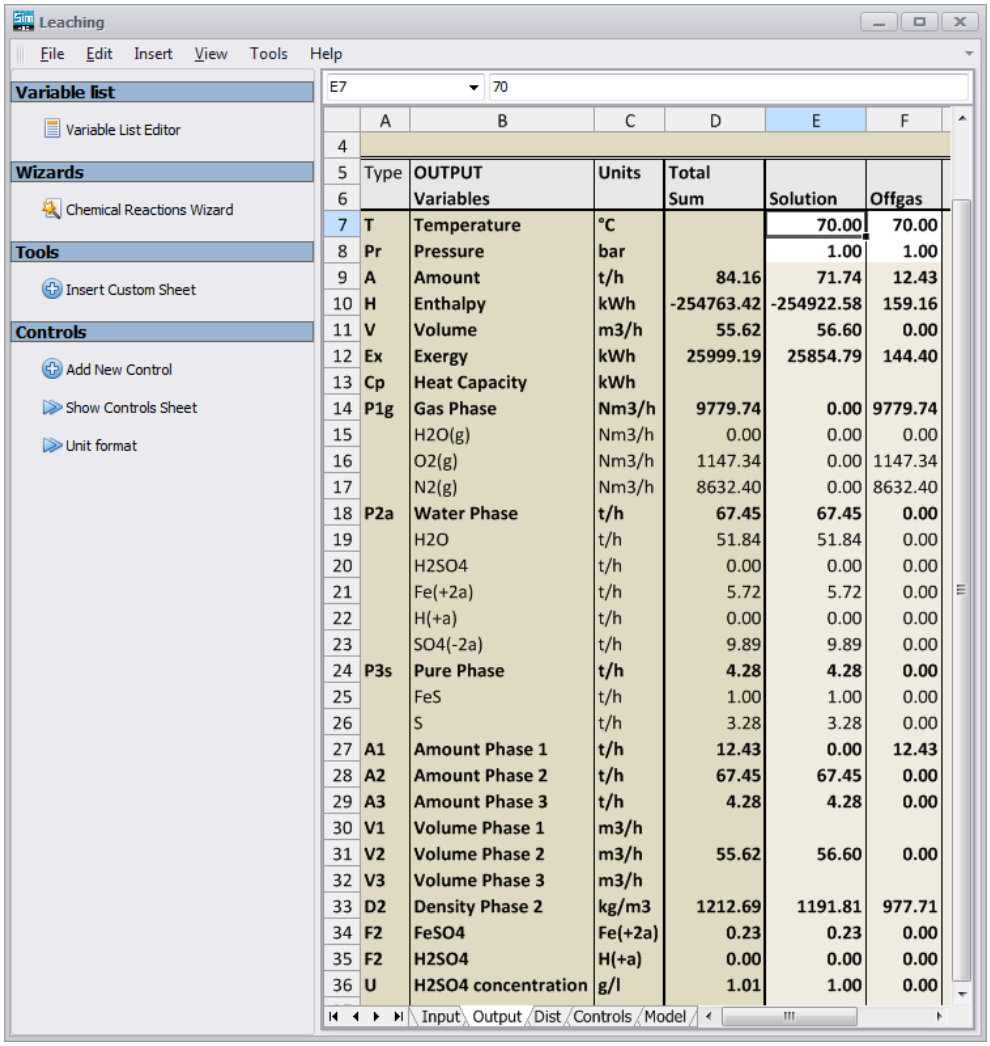
Output sheets of both Leaching and Cooler units:

- Temperature of solution and offgas streams should be set to 70 °C, see **Fig. 12**.
- Temperature of hot water stream should be set to 60 °C.



	A	B	C	D	E	F	G
4							
5	Type	INPUT	Units	Total			
6		Variables		Sum	FeS	H2SO4	Air
7	T	Temperature	°C		25.00	25.00	25.00
8	Pr	Pressure	bar		1.00	1.00	1.00
9	A	Amount	t/h	84.16	60.00	10.10	14.06
10	H	Enthalpy	kWh	-246798.99	-223520.49	-23278.49	0.00
11	V	Volume	m3/h	60.11	50.15	10.13	0.00
12	Ex	Exergy	kWh	33512.47	28640.61	4681.93	189.93
13	Cp	Heat Capacity	kWh				
14	P1g	Gas Phase	Nm3/h	10927.08	0.00	0.00	10927.08
15		H2O(g)	Nm3/h	0.00			
16		O2(g)	Nm3/h	2294.69			2294.69
17		N2(g)	Nm3/h	8632.40			8632.40
18	P2a	Water Phase	t/h	60.10	50.00	10.10	0.00
19		H2O	t/h	50.00	50.00		
20		H2SO4	t/h	10.10		10.10	
21		Fe(+2a)	t/h	0.00			
22		H(+a)	t/h	0.00			
23		SO4(-2a)	t/h	0.00			
24	P3s	Pure Phase	t/h	10.00	10.00	0.00	0.00
25		FeS	t/h	10.00	10.00		
26		S	t/h	0.00			
27	A1	Amount Phase 1	t/h	14.06	0.00	0.00	14.06
28	A2	Amount Phase 2	t/h	60.10	50.00	10.10	0.00
29	A3	Amount Phase 3	t/h	10.00	10.00	0.00	0.00
30	V1	Volume Phase 1	m3/h				
31	V2	Volume Phase 2	m3/h	60.11	50.15	10.13	0.00
32	V3	Volume Phase 3	m3/h				
33	D2	Density Phase 2	kg/m3	999.80	996.95	996.95	996.95
34	F2	FeSO4	Fe(+2a)	0.00	0.00	0.00	0.00
35	F2	H2SO4	H(+a)	0.00	0.00	0.00	0.00
36	U	H2SO4 concentration	g/l	0.00	0.00	0.00	0.00

Fig. 11. Feed stream amounts of the Leaching unit.



	A	B	C	D	E	F
4						
5	Type	OUTPUT	Units	Total		
6		Variables		Sum	Solution	Offgas
7	T	Temperature	°C		70.00	70.00
8	Pr	Pressure	bar		1.00	1.00
9	A	Amount	t/h	84.16	71.74	12.43
10	H	Enthalpy	kWh	-254763.42	-254922.58	159.16
11	V	Volume	m3/h	55.62	56.60	0.00
12	Ex	Exergy	kWh	25999.19	25854.79	144.40
13	Cp	Heat Capacity	kWh			
14	P1g	Gas Phase	Nm3/h	9779.74	0.00	9779.74
15		H2O(g)	Nm3/h	0.00	0.00	0.00
16		O2(g)	Nm3/h	1147.34	0.00	1147.34
17		N2(g)	Nm3/h	8632.40	0.00	8632.40
18	P2a	Water Phase	t/h	67.45	67.45	0.00
19		H2O	t/h	51.84	51.84	0.00
20		H2SO4	t/h	0.00	0.00	0.00
21		Fe(+2a)	t/h	5.72	5.72	0.00
22		H(+a)	t/h	0.00	0.00	0.00
23		SO4(-2a)	t/h	9.89	9.89	0.00
24	P3s	Pure Phase	t/h	4.28	4.28	0.00
25		FeS	t/h	1.00	1.00	0.00
26		S	t/h	3.28	3.28	0.00
27	A1	Amount Phase 1	t/h	12.43	0.00	12.43
28	A2	Amount Phase 2	t/h	67.45	67.45	0.00
29	A3	Amount Phase 3	t/h	4.28	4.28	0.00
30	V1	Volume Phase 1	m3/h			
31	V2	Volume Phase 2	m3/h	55.62	56.60	0.00
32	V3	Volume Phase 3	m3/h			
33	D2	Density Phase 2	kg/m3	1212.69	1191.81	977.71
34	F2	FeSO4	Fe(+2a)	0.23	0.23	0.00
35	F2	H2SO4	H(+a)	0.00	0.00	0.00
36	U	H2SO4 concentration	g/l	1.01	1.00	0.00

Fig. 12. Output stream temperatures of both Solution and Offgas streams are put at 70 °C.

44.2.7. Saving the Process, Chapter 40 (sections 40.2. and 40.3.1.)

Processes should always be saved in their own folder. Changing the process name is not enough since every unit is an Excel file that is saved in the same folder as the flowsheet. The name of these files is the same as the name of the units. Therefore you also have to save different scenarios in different folders.

44.2.8. Running the Simulation and Checking the Results, sections 40.3.1 and 40.3.2

When you have finished the model you can run the simulation. First you have to set the number of rounds you wish to calculate the process and then press the Simulate button to start the simulation. You should check if the values change during different runs to find out if the process is in balance. The value of the selected variable is presented in the value labels, see **Fig. 13**. User can add Stream Tables and Header (Chapter 40 sections 40.1.4 and 40.3.1) to visualize the calculation results, see **Fig. 14** and **Fig. 15**.

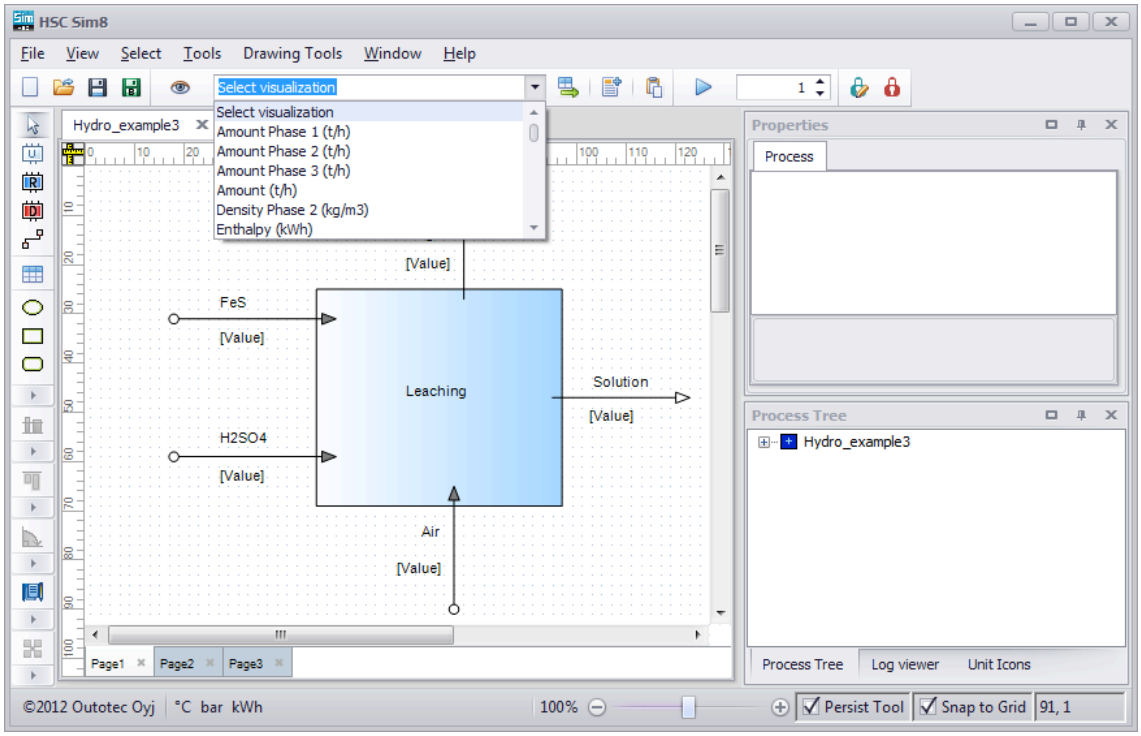


Fig. 13. Selecting visualization from the list.

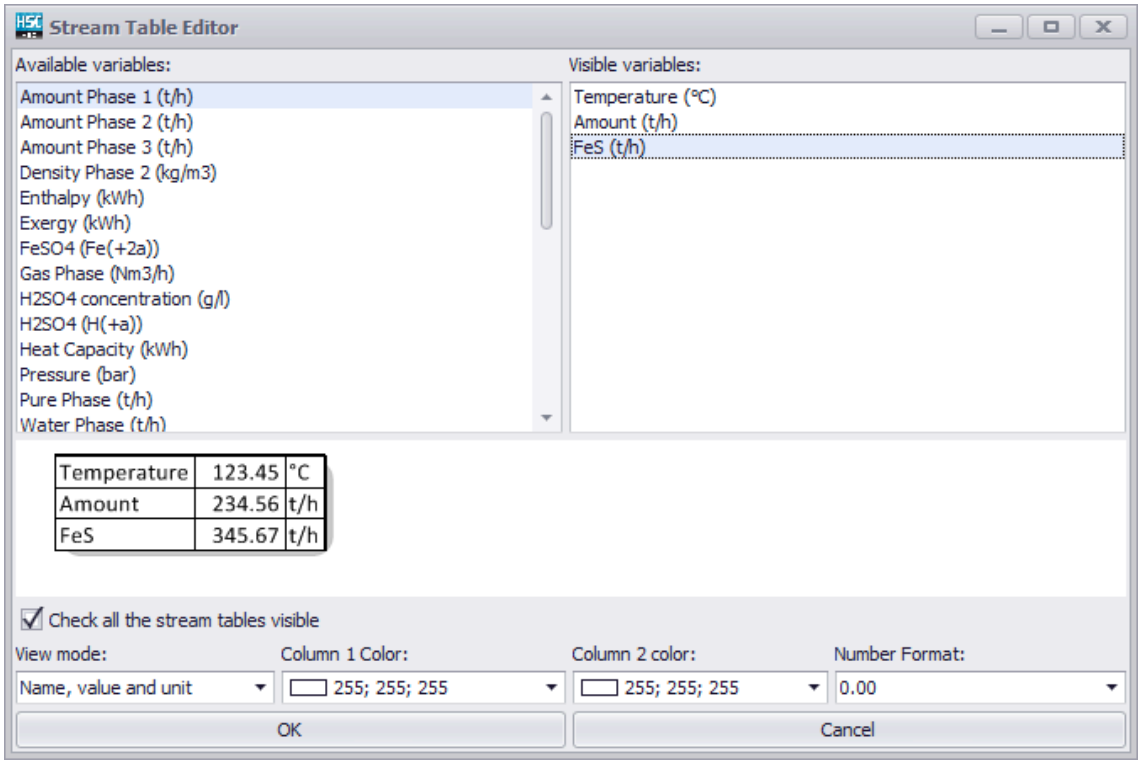


Fig. 14. Stream Table Editor to modify Stream Tables.

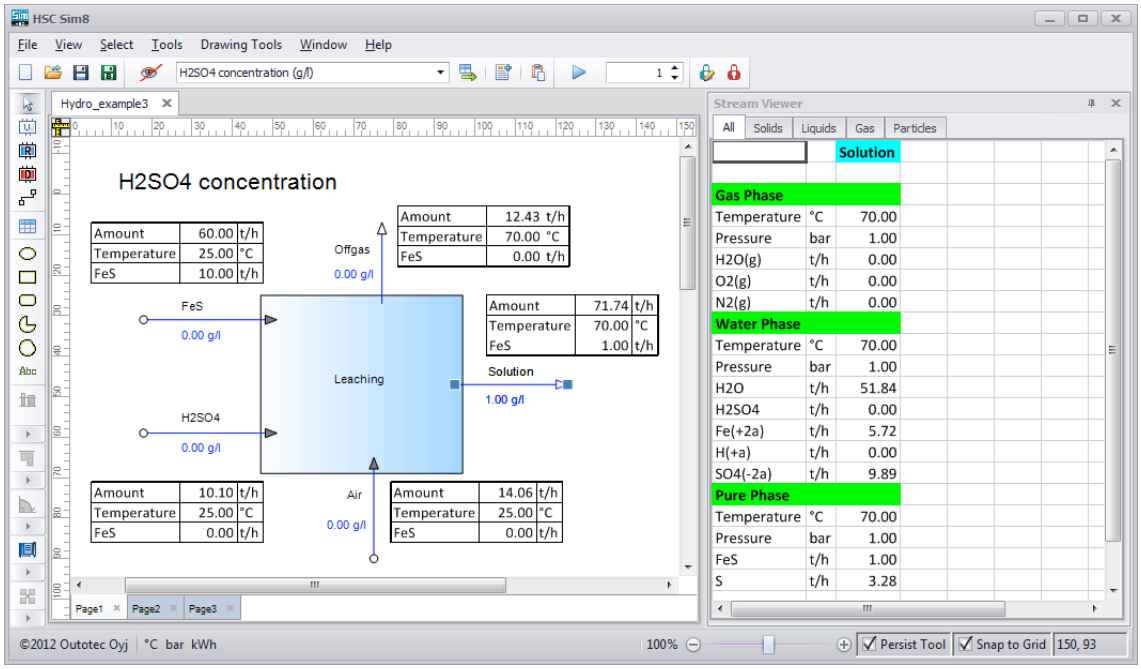


Fig. 15. Stream Tables and Stream Viewer to visualize calculation results.