

41. Sim Reactions Example

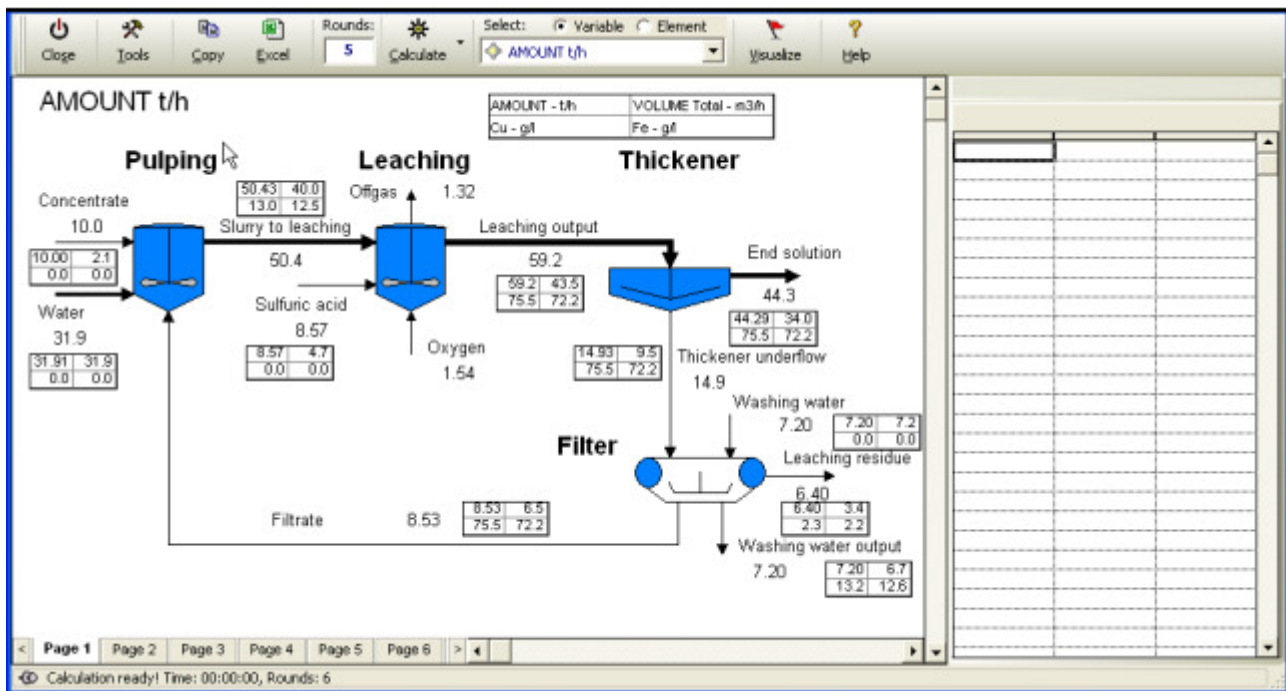


Figure 1: Sim Reactions Example, Run mode view after calculations.

General

This example contains instruction how to create a simple model. The example is a hydrometallurgical process and the same basic ideas may also be used in other areas. The example files can be found from the HSC Chemistry installation folder ...Flowsheet_Hydro\Example Reactions\Example Reactions.flx. This describes the creation of the example in detail with references to the Sim Flowsheet manual. However, there is no need to do everything in the same order as described below.

Drawing a flowsheet, see Chapter 40.5

- Select the unit icons from the Properties toolbar, Units sheet. If you need to modify the unit icons, see Chapter 40.5.2. If you modify or copy the units, remember to change the object type to Unit since the pasted objects are always of the Drawing type, see Chapter 40.3.2 Properties toolbar.
- Draw the streams between the units. One mouse click for the start and to the corners and double click to the end. If the units are Unit-type objects and the stream touches the unit then the source and destination is automatically filled for the stream. For editing the stream afterwards please see Chapter 40.5.1.
- Name the units and streams see Chapter 40.3.2.
- Add the necessary labels. For example, a header label and value labels. Chapter 40.3.14.
- Check the source and destination for the streams. This can be done with Overlay and Route check –tool, Chapter 40.3.13.
- If you need to change the format of the labels or names in the flowsheet you can select all the same kind of labels or names with Edit – Select tool, see Chapter 40.3.1.

Setting the global measure units, see Chapter 40.6

You find this tool from Excel editor from the bottom-right corner of the window. In this case the default units are correct.

Setting the variable list, see Chapter 40.6

The sample variable list is used as a base list in this example. You can add the list to the model from the Variable type selection tool (In Excel editor, Tools menu, Variable Type) by pressing the “Sample variable list” button, Figure 2. You may also fill the variable list manually; the Variable Type Dialog may be used to select the available types for the variables.

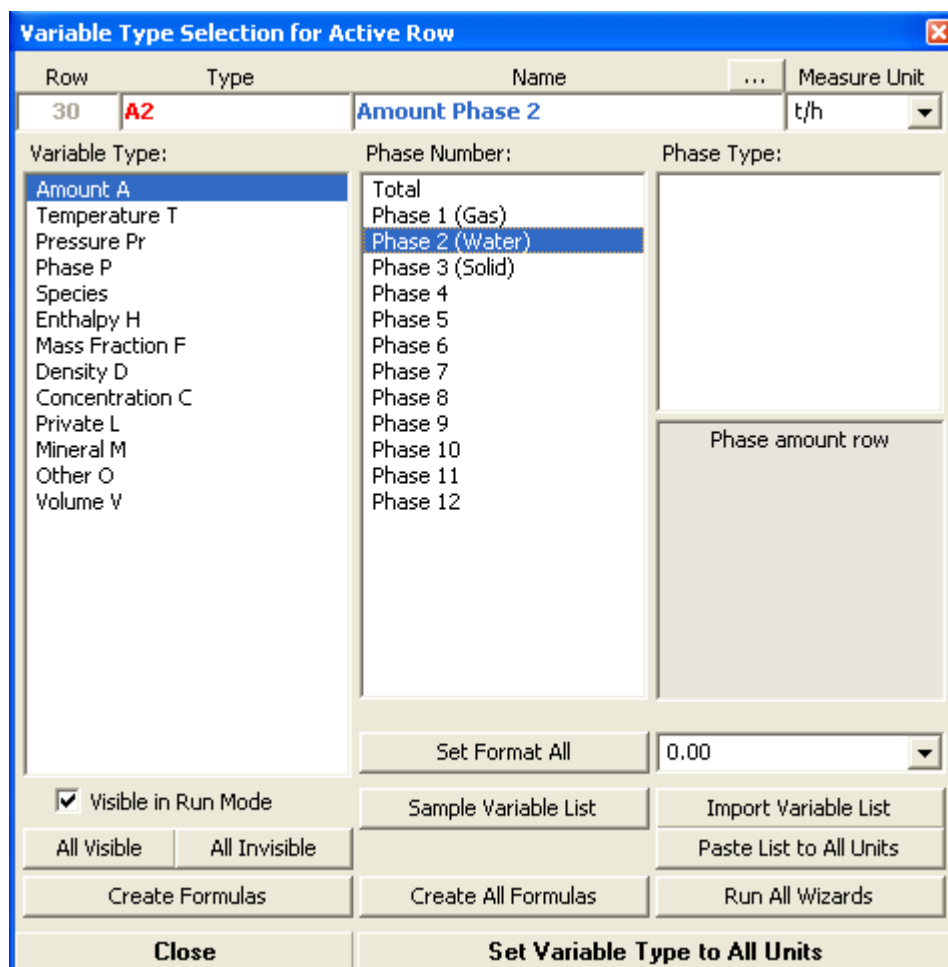


Figure 2: Variable type selection window.

You are not limited into the variable types available in the Variable Type dialog, Figure 2. However, if you create your own variable types (Type: Other O in A column) you must create also the possible formulas manually. For example, "Solid concentration" is not in the sample list and it may be added to the bottom of the list.

- Open any unit in Excel editor and select the input or output sheet.
- Write the type of the variable to the A column (O), name of the variable to the B column (Solid concentration) and unit of the variable to the C column (g/l).

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- Make the formula to the D column. In the example the formula is $D31/D47*1000$, which means that the total solid mass is divided by the total slurry volume and the result is multiplied by 1000 to get the unit to grams solid per liter slurry.
- Copy this formula to the columns E, F and G. These three columns are enough in the example since the maximum number of input or output streams in one unit is three.
- Copy the formula to the other units with the Global cell editor, Chapter 40.16. Open the Cell editor from Excel editor – Tools – Cell editor... Select the first cell where the previously-made formula is and press the Enter button in the Cell editor window. Do the same for all three cells that have the formula. After that the formula is in every unit in input and output sheets. Please see Figure 3.

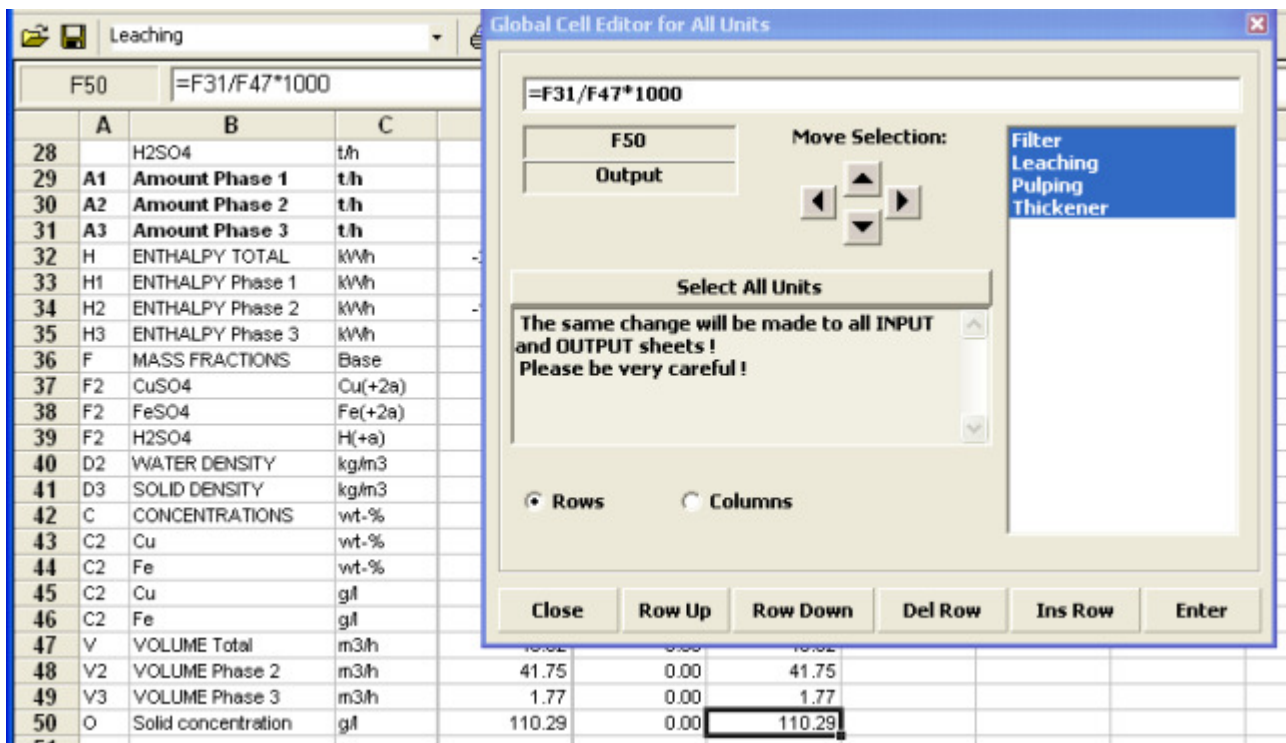


Figure 3: The Global cell editor.

Solid density, as well as liquid density, is filled automatically if you use automatic formula creation. These can be filled manually if you change the variable (text in A column) from D2 to D2m. In the example it is filled automatically.

When modifying the variable list, remember that the columns A to D are automatically synchronized, which means that any changes are automatically copied to all units in the process. Chapter 40.2.3.

Create the formulas for the variables from the Variable type selection – Create All Formulas button (or Recreate Formulas to All Process Units button in Global measure units window), Figure 2. This creates the formulas for variables according to the variable type in column A.

Add reaction equations to the unit, Chapter 40.7.2

The reaction equations can be added with the Distribution wizard. Choose the leaching unit and open the Excel editor and select "Wizard – Chemical reaction model..." You only have to write the compounds and press the Balance button, which adds the coefficients for the reactions. In the example the reactions are as presented in Figure 4.

No	Progress %	Reactants	Products	Balance	H kcal/mol	K 25 °C
1	80	2 CuS + 2 H2SO4 + O2(g)	= 2 Cu(+2a) + 2 H2O + 2 SO4(-2a) + 2 S	OK	-125.91	3.56E+060
2	80	2 FeS + 2 H2SO4 + O2(g)	= 2 Fe(+2a) + 2 H2O + 2 SO4(-2a) + 2 S	OK	-178.63	1.28E+099
3	3	H2O	= H2O(g)	OK	10.52	3.16E-002

Figure 4: Reactions sheet in Distribution wizard.

	A	B	D	E	F	G
1	DISTRIBUTIONS		Total	Output Streams %		
6	Phases / Species		%	Offgas	Leaching output	
7	A	AMOUNT	0.00			
8	T	TEMPERATURE	0.00			
9	Pr	PRESSURE	0.00			
10	P1	GAS PHASE	100.00	100.00	0.00	
11		N2(g)	0.00			
12		O2(g)	0.00			
13		H2O(g)	0.00			
14		SO2(g)	0.00			
15		H2S(g)	0.00			
16	P2	WATER PHASE	100.00	0.00	100.00	
17		H2O	0.00			
18		H(+a)	0.00			
19		OH(-a)	0.00			
20		Cu(+2a)	0.00			
21		Fe(+2a)	0.00			
22		Mg(+2a)	0.00			
23		SO4(-2a)	0.00			
24	P3	PURE SUBSTANCES	100.00	0.00	100.00	
25		CuS	0.00			

Figure 5: Distributions sheet in Distributions wizard.

Remember also to complete the Distributions sheet! It is the same as the Distribution model, Chapter 40.7.1. In the example 100% of gas phase go to the Off gas stream and 0% of liquid and solid phase. Fill in the percentage for both streams, i.e. rows 10, 16 and 24 in the example. Press the Apply button to accept the changes for both sheets, Figure 5.

In the pulping reactor there are no reactions and only one output stream. The easiest way to make the formulas for the output sheet is with the Distribution wizard. Fill in the rows where there are phase names as described above. Of course you can make the formulas on the output sheet by yourself. In this case, the formula would be the link to the same row in the D column of the input sheets.

Load and run Excel wizards for the thickener and the filter, Chapter 56

You may create the unit models manually like in Excel, however, the Wizards usually offer an easier way. For the thickener and filter an example wizard is available. You can load it from the Excel editor with selection "Wizard, Load Excel wizards...". This will open a new window where you can load and apply wizards to the units.

Loading the wizard will only copy it onto the wizard sheet into the unit. Applying the wizard will make changes to the unit. In this case when you apply the wizards you are asked to select different streams in the input or output columns. This is because the streams can be in different columns depending in which order you have drawn them or they might have different names if you use for example other language than English.

You can always rerun the wizard. Wizard-sheet do not carry out calculations, it may be needed to recreate the unit model onto the Model-sheet. For more detailed instructions about the loading and applying wizards please see Chapter 56.

Setting controls to the process, Chapter 40.13

In the example the solid concentration after the pulping reactor is controlled to 250 g solids/liter of slurry. The control is made to the units control sheet. The control sheet is presented in Figure 6. The following rows are filled in.

Table 1. The feed data for controlling the solid concentration after pulping. Please note that the streams can be in different order in the Input sheet. The cell reference is wanted for the water input stream.

The row name (Cell)	Filled value or formula	Notes
Set point (C7)	250	Desired solid concentration, g/l
Measured (C8)	=Output!E50	Measured solid concentration, g/l
Tolerance +/- (C9)	1	Tolerance for the concentration
Value (C14)	=Input!F17	Water input to the process, t/h
X Min Limit (C15)	0	Minimum amount for Value cell
X Max Limit (C16)	100	Maximum amount for Value cell

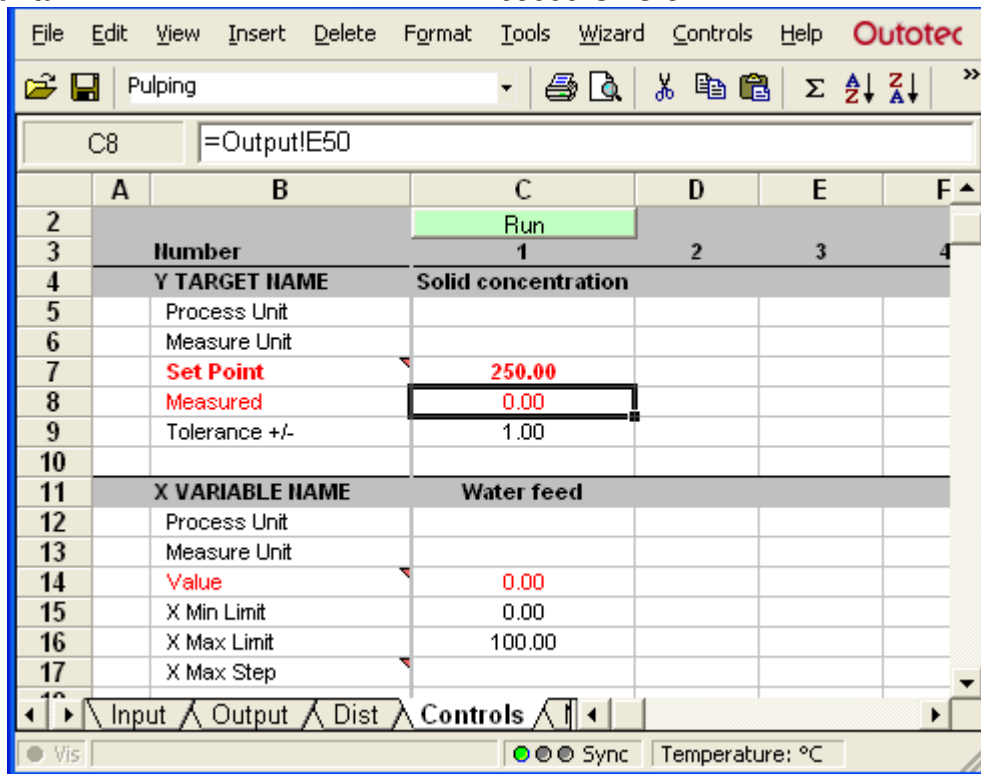


Figure 6: The controls sheet of the pulping.

The other control is needed to the leaching to adjust the amount of sulfuric acid fed to the process. In this case we assume that the acid is fully consumed in the leaching.

Table 2. The feed data for controlling the sulfuric acid feed for the leaching. In this case the desired amount of acid in the output stream should be equal with the tolerance, then we avoid negative values. If the Set Point were null then the accepted values according to the Tolerance would be from -0.001 to 0.001 .

The row name (Cell)	Filled value or formula	Notes
Set point (C7)	0.001	Desired amount of acid in output, t/h
Measured (C8)	=Output!F28	Measured amount of acid in output, t/h
Tolerance +/- (C9)	0.001	Tolerance for the acid amount
Value (C14)	=Input!F28	Acid input to the process, t/h
X Min Limit (C15)	0	Minimum amount for Value cell
X Max Limit (C16)	100	Maximum amount for Value cell

Setting feed streams for the process

All feed streams to the process should be set. If the feed to the process is not set the stream is ignored. We have already set some feed streams.

- Washing water for filter is set when we used the wizard for the unit.
- Water feed is set to be dependent on the solid feed to the pulping with the control.
- Sulfuric acid feed is dependent on the acid consumption in the leaching, also set with the control.

The concentrate feed in the example is set to 5 t/h CuS and 5 t/h FeS, Figure 7. Fill in these values to the input sheet of the pulping unit, rows 25 and 26. The correct column is the one that has the right name in row 6. If you have problems to get the correct name to row 6, check that you have the correct destination in the stream information. Properties toolbar – Process sheet – Destination, see Properties toolbar in the Chapter 40.5. To refresh the information in the row 6 select Excel editor – Tools – Refresh.

1	Pulping							NOTE: Formulas cannot be used on columns E ->
2	Authors:							
3	Date:							
4	INPUT STREAMS							
5	Type	INPUT Variables	Units	Total Sum	Concentrate	Water	Filtrate	
7	A	AMOUNT	t/h	10.00	10.00	0.00	0.00	
8	T	TEMPERATURE	°C					
9	Pr	PRESSURE	bar					
10	P1g	GAS PHASE	t/h	0.00	0.00	0.00	0.00	
11		N2(g)	t/h	0.00				
12		O2(g)	t/h	0.00				
13		H2O(g)	t/h	0.00				
14		SO2(g)	t/h	0.00				
15		H2S(g)	t/h	0.00				
16	P2a	WATER PHASE	t/h	0.00	0.00	0.00	0.00	
17		H2O	t/h	0.00				
18		H(+a)	t/h	0.00				
19		OH(-a)	t/h	0.00				
20		Cu(+2a)	t/h	0.00				
21		Fe(+2a)	t/h	0.00				
22		Mg(+2a)	t/h	0.00				
23		SO4(-2a)	t/h	0.00				
24	P3	PURE SUBSTANCES	t/h	10.00	10.00	0.00	0.00	
25		CuS	t/h	5.00	5.00			
26		FeS	t/h	5.00	5.00			
27		S	t/h	0.00				
28		H2SO4	t/h	0.00				
29	A1	Amount Phase 1	t/h	0.00	0.00	0.00	0.00	
30	A2	Amount Phase 2	t/h	0.00	0.00	0.00	0.00	
31	A3	Amount Phase 3	t/h	10.00	10.00	0.00	0.00	

Figure 7: You must specify the input stream amounts and temperatures on the Input-sheet. You should fill only the streams that are coming outside to the process. Intermediate streams are filled automatically when the process is calculated.

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Oxygen feed is the last feed stream in our example. In the example, oxygen is fed to the process 1.1 times the amount required. The formula made to the oxygen feed column (check the row 6 described above) in the input sheet is: =ABS(Model!F12)*1.1

Saving the process, Chapters 40.2.6 and 40.2.7

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

Running the simulation and checking the results, Chapter 40.9 and 40.9.1

When you have finished the model you can run the simulation. To run it you have to go to the Run mode, Run – Start simulation or F5. First, you have to set how many rounds you calculate the process and then press the Calculate button to start the simulation. You should check if the values change during different runs to find out if the process is in balance or you can use End criteria. Then you have the results and you can select a variable from the Variable selection box. The value of the selected variable is presented in the value labels. Please see Figure 1.

Adding stream tables, Chapter 40.5.3

To show multiple variables a stream table can be added for the streams. In this case default 2x2 table is added for all streams and presented variables are: Total volume (m³/h), Total mass (t/h), Cu concentration (g/l) and Fe concentration (g/l). The stream tables are put to other layer and then they can easily be hidden. Next is explained how to do the changes.

1. Select all streams and add tables to streams, Select menu, Streams and Tools menu, Insert Table. Insert also the Header Table for the Tables, Tools menu, Insert Stream Header Table.
2. Then the variables are added to tables: Edit one table with mouse left double click, add variables by selecting Edit menu, Variables or pressing Add Variable button. You may also edit the formatting of the table. To copy size or formatting changes to all tables use Apply formatting to all tables tool in Format menu in Edit Table window.
3. You may put tables to separate layer: Select all tables, Select menu, Select Stream Tables. Add also the Stream Header Table to the selection by selecting it with Shift key pressed. Then change the layer property on properties toolbar on left to Layer 1. Now you can hide all tables if you deselect layer 1 from View menu, Layers.

Useful tools to manage the model

Here are briefly presented a few of the tools provided with HSC-Sim that make the creation of the models easier. These tools are needed in virtually every simulation model.

Global Cell Editor, Chapter 40.16

- If you need the variables that are not present in the Variable type selection, this is the easiest way to copy them to all units.

Variable Type Selection, Chapter 40.6

- It is advised to use ready-made variables when possible.

Distribution Wizard, Chapter 40.7.2 and Excel wizards, Chapter 56

- With wizards you can easily make a new unit.

Element Balances, Chapter 40.11

- This tool is useful for checking if there are any balance errors in the process.

Find Errors, Chapter 40.9

- This tool checks the element balances, errors in controls and other common problems.
- All is collected to one window.