

11. Heat and Material Balance Module

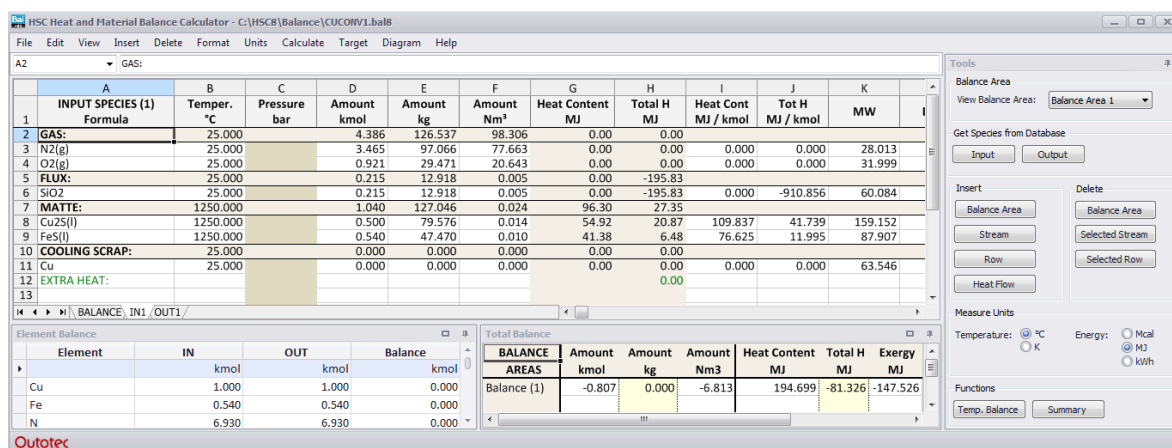


Fig. 1. Heat and Material Balance workbook with BALANCE, IN1 and OUT1 sheets.

Heat balance calculations are usually carried out when developing new chemical processes and improving old ones, because no process can work if too much heat is released or if there is a lack of thermal energy to maintain the reaction temperature. This module calculates the real or constrained heat balances, with given mass balances as the boundary conditions, but not the theoretical balances at equilibrium conditions.

The heat balance application always contains BALANCE, IN1, and OUT1 sheets. A pair of IN and OUT sheets is called a *Balance area*, which may be considered equivalent to a control volume. Many balance areas may be inserted, to create a multiple balance area workbook. Multiple balance area workbooks are explained in more detail in Section 11.9. Multiple balance areas. For the sake of simplicity, only the first balance area (IN1, OUT1) will be described in the following chapters.

The basic idea of the heat balance module is that the user specifies the IN1 and OUT1 species, temperatures and amounts and the Heat Balance module *automatically* calculates the heat and material balances using the BALANCE sheet. The Heat balance module updates the calculated results on the BALANCE row at the bottom of the form each time the user changes the input data. **Please do not modify the BALANCE sheet.**

Since the program uses and creates new balance areas according to the names of the sheets, it is extremely important that *the automatically created sheet names, i.e. the BALANCE, INx and OUTx sheets, should not be modified.*

You can also add new sheets for other spreadsheet calculations using the **Insert Sheet** and **Insert Excel Sheet** selections in the menu. The other sheets work very much like MS Excel worksheets, for example, you can:

- rename the sheet name by double clicking the sheet tab
- type formulae into the cells
- use similar cell references as in Excel
- use most of the Excel functions
- link the sheet to the IN1 sheet using normal Excel cell references, for example, for converting elemental analysis of the raw material into component amounts.
- use the heat balance calculation results in the OUT1 sheet as the initial values for other spreadsheet calculations.

In addition, the Heat Balance menu provides a wide range of Excel type features, such as: number, font, alignment and border formatting, defined name settings, and cell protection. Because they are not necessarily needed in heat balance calculations, these features are not described here in detail.

The new heat balance module offers several ways to calculate heat and material balances:

1. The user types the input and output species, temperatures and amounts into the IN1 and OUT1 sheets respectively. This is a simple way to calculate heat and material balances.
2. Materials (species) are given as groups of substances, called *streams*. These streams can be the same as the phases, but they can also be a mixture of phases.
3. The output amounts can be linked with the input amounts with Excel-type cell references, or vice versa.

11.1. Basic Calculation Procedure

The following procedure will describe the most simple way to calculate Heat Balance:

1. Enter the input substances (raw materials), temperatures and amounts into the IN1 sheet. It is possible to either type amounts in kmol, kg or Nm³. *It is advised to use **kmol** and **kg** because missing density data may cause inaccuracy with Nm³ units.*
2. Enter the output substances (products), temperatures and amounts into the OUT1 sheet. Type the amounts in either kmol, kg or Nm³ as preferred.
3. When feeding additional energy (electricity) to the process, enter the amount into the **Total** column in the last empty row of the IN1 sheet. You can also type for example "Extra Heat" in the first column of this row, see **Fig. 1**. The Database module will convert the color of all "inert" text in the first column to green, unless this text is identified in the database as a substance. Note that:

$$1 \text{ kWh} = 3.6 \text{ MJ} = 0.8604 \text{ Mcal (th)}.$$

However, the Balance module will automatically recalculate the green text when changing the units from the menu. If the green text cell contains a formula, it will *automatically be changed according to the new unit*. For example, a change from °C to K will add "+ 273.15" to the end of the formula.

4. If heat loss values are known, then type them into the last empty row of the OUT1 sheet in the last column (**Total**). A first estimate of heat losses for an air-cooled reactor (natural convection) can easily be calculated using the following formula in **kcal/h**:

$$H_{\text{loss}} = (6.8 + 0.046 * T_2) * (T_2 - T_1) * A \quad (1)$$

where: A = Outer surface area of the reactor (m²)
T₂ = Surface temperature of the reactor (°C)
T₁ = Room temperature (°C)

Please use the Heat Loss module if more accurate heat loss approximations are required.

5. HSC automatically and immediately updates the heat balance on the bottom line as soon as changes to any input data are made.
6. HSC also automatically updates the material amount balances in mol, kg and Nm³ units. Note that only the mass balance in kg units on the bottom row should be zero; the mole or volume balances can easily change in any chemical process.
7. The element balance can be checked from **Element Balance**, see **Fig. 1**.
8. By selecting **Temperature Balance** from the **Calculate** menu or from the **Temp. Balance** button, it is possible to see the estimated temperature of the products when the heat balance = 0, see **Fig. 1** and **Fig. 2**.

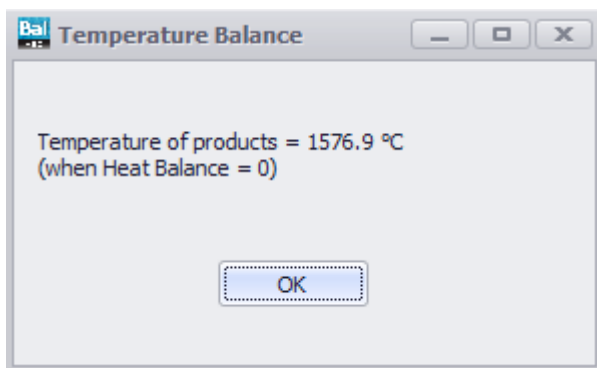


Fig. 2. Temperature of products (adiabatic process).

9. To insert an empty row in the table, select **Row** from the **Insert** menu or by pressing the right mouse button and selecting **Insert Row** from the popup menu.
10. Rows can be deleted by selecting **Row** from the **Delete** menu or pressing the right mouse button and selecting **Del Row** from the popup menu.
11. You can change the order of the substances by inserting an empty row and using the Copy - Paste method to insert the substance in the new row. The Drag and Drop method can also be used. **However, it is extremely important to Copy and Paste the whole row, not only the formula, because of auxiliary data in the hidden columns on the right side of the IN1 and OUT1 sheets.**
Please keep the **Copy Mode** selection **on** in the **Edit** menu when rearranging the species, as this will force the program to select the whole row. When formatting the columns and cells, turn the **Copy Mode** selection **off** in the **Edit** menu.
12. Temperature units can be changed by selecting the °C or K from the **Tools bar** or **Units menu**.
13. Energy units can be changed by selecting **Mcal**, **MJ**, or **kWh** from the **Tools bar** or **Units menu**.
14. If a paper copy is needed, select **Print** from the **File** menu. This option will copy all the data onto the same print sheet and will also print this sheet on paper if the user presses OK. Notice that you can delete this print sheet by activating it and then selecting **Sheet** from the **Delete** menu. The **Print Sheet** selection in the **File** menu will print only the active sheet.
15. To save the sheets, select **Save** from the **File** menu. Please save the sheets often using different names, because you may wish to make small changes later or to return to the original sheet. Saving sheets is important, because the Undo feature is not available in HSC Chemistry.
16. It is possible to take into account the water/steam pressure compensation by moving the cursor to an H₂O or H₂O(g) species and selecting *Insert/Pressure correction H₂O* from the menu. This allows user to type pressure in column C, which is otherwise non-editable. This is useful when calculating steam processes, for example.

11.2. Formatting the Worksheet

The heat balance module offers several Excel-type formatting possibilities. These may be selected in the **Format** menu:

- Number, Font, Font Default, Alignment, Border, Pattern, Object (for graphical objects), Sheet, Options
- Column Width, Row Height
- Define Names, Refresh Names
- Protection On, Off, Lock all Cells, Unlock all Cells

The window size may also be changed from the **View** menu. **Normal** gives a VGA size window, **Full Height** uses the whole height of the screen, and **Full Width** fills the whole screen.

11.3. Specification of Substance Groups (Streams)

HSC Chemistry 8.0 offers the possibility to specify the input and output substances in streams. These streams can be made of one or several physical phases or species which have the same fixed temperature and elemental composition. Although heat and material balance calculations can be made without using streams, division into streams helps considerably when changing temperatures and material amounts. Notice that when using *formulae/links in temperature cells, the temperature cells are not updated unless the species are divided into streams.*

Some examples of “one-phase streams” are:

1. Air feed.
2. Process gas output.
3. Homogenous liquid and solid inputs and outputs.

Some examples of “multi-phase streams” are:

1. Liquid material with solid particles (suspension) as input or output.
2. Solid feed mixture of the process, made of different substances such as mineral concentrate, coal. and sand.
3. Gas feed with liquid droplets or solid powder.

The species rows in the IN1 and OUT1 sheets are divided into separate groups by special stream rows. These rows can be inserted in the sheet using the **Stream** selection in the **Insert** menu or using the same selection in the popup menu from the right mouse button.

The heat balance module *automatically* makes the following modifications to the sheet when you insert a new stream (group) row in the sheet:

1. Asks for a name for the new group, which you can change later if necessary.
2. Inserts a new empty row above the selected cell with a light blue pattern.
3. HSC assumes that all rows under the new group row will belong to the new group down to the next group row.
4. Inserts Excel-type SUM formulae in the new group row for calculating the total amount in the group using kmol, kg, and Nm³ units.

Once the insert procedure is ready, you can edit the group row in the following way:

1. The stream name (label) can be edited directly in the cell.
2. The stream temperature can also be changed directly in the cell and will affect the temperature of all the species in this group.
3. The total material amount of the group can be changed simply by typing a new amount in the group row in kmol, kg, or Nm³ units. This amount can be typed directly over the SUM formula and the program will automatically change the amounts of the species, keeping the overall composition constant. The program will then regenerate the original SUM formula after calculating the new amounts.
4. It is important to note that you are unable to type formulae in the amount and enthalpy columns of the stream row, because the SUM formulae must be in the stream row.

To change the amounts of species in a stream using kmol, kg, or Nm³ units, simply type the new amount in the corresponding cell. The program will automatically update the amounts in the other columns, the total amount of the stream, and the total material and heat balance as well.

An example of species streams can be seen in **Fig. 3**. The output species have been divided into four streams. In this example the species in each stream exist in the same phase. **Process Gas** is a gaseous mixture phase, **Slag** is a molten mixture phase, and **White Metal** is a pure molten substance.

A	B	C	D	E	F	G	H	I	J	K
OUTPUT SPECIES (1)	Temper.	Pressure	Amount	Amount	Amount	Heat Content	Total H	Heat Cont	Tot H	MW
Formula	°C	bar	kmol	kg	Nm ³	MJ	MJ	MJ / kmol	MJ / kmol	
1										
2	1250.000		4.082	135.121	91.496	174.73	5.25			
3	1250.000		3.465	97.066	77.663	135.87	135.87	39.212	39.212	28.013
4	1250.000		0.046	1.477	1.035	1.91	1.91	41.458	41.458	31.999
5	1250.000		0.571	36.578	12.798	36.95	-132.53	64.709	-232.104	64.059
6	1300.000		0.283	56.738	0.013	64.75	-274.64			
7	1300.000		0.215	43.812	0.010	50.05	-248.03	232.782	-1153.638	203.777
8	1300.000		0.037	8.490	0.002	10.75	-26.52	293.250	-723.294	231.539
9	1300.000		0.031	4.436	0.001	3.95	-0.09	127.390	-2.831	143.091
10	1250.000		0.469	74.642	0.013	51.51	19.58			
11	1250.000		0.469	74.642	0.013	51.51	19.58	109.837	41.739	159.152
12	1250.000		0.000	0.000	0.000	0.00	0.00			
13	1250.000		0.000	0.000	0.000	0.00	0.00	40.234	48.262	63.546
14	1250.000		0.000	0.000	0.000	0.00	0.00			

Element	IN	OUT	Balance
Cu	1.000	1.000	0.000
Fe	0.540	0.540	0.000
N	6.930	6.930	0.000

Fig. 3. The OUT1 sheet of the Heat Balance module. The species have been divided into three streams, which are the same as the existing phases.

11.4. Formulae in the Cells

Excel-type formulae and cell references can be used, for example, in order to link the input and output amounts with each other and to maintain the material balance automatically when the input amounts change. The input and output amounts can be linked using two main methods:

1. An Excel-type formula can be typed in the **kmol column**, which expresses the dependence of the output mole amount on the input mole amount. For example, if the Cu₂S in the cell OUT1!C10 contains 93.8 % of copper input then you can type the formula **= 0.938*IN1!C7** in cell OUT1!C10, see **Fig. 4**.
2. The Heat Balance module automatically calculates the input and output mole amounts for elements. The cell names for input amounts are: InAc, InAg, InAl, InAm and the equivalent for output elements are called OutAc, OutAg, OutAl, OutAm, etc. For balance areas with a higher number (for example the IN2 and OUT2 sheets) the corresponding cell names are simply InAc2, InAc3 and OutAc2, OutAc3, etc. These names can be used in the formulae. The formula in the previous example can also be written: **=0.938*(InCu-C12)/2** using these defined names, see **Fig. 5**. The cells with element amounts are not visible to the user.

Please be very careful when using default input and output names simultaneously, because it is very easy to end up with circular references. An indication of a circular reference is that the heat and material balance, which can be seen on the BALANCE row, changes even after a recalculation (**Calculate/ReCalc** from the menu). By selecting **Format/Options** from the menu and highlighting the **Iteration** checkbox under the **Calculation** tab, it is possible to iterate circular references automatically. This is, however, not recommended for very large worksheets.

In the IN1 and OUT1 sheets, it is recommended to use formulae only in the kmol column and not in the other Amount columns. You can also use the formulae in other columns, but please be very careful. In the other sheets there are no special limitations for the formulae.

	A	B	C	D	E	F	G	H	I	J	K
	OUTPUT SPECIES (1)	Temper.	Pressure	Amount	Amount	Amount	Heat Content	Total H	Heat Cont	Tot H	MW
	Formula	°C	bar	kmol	kg	Nm ³	MJ	MJ	MJ / kmol	MJ / kmol	
2	PROCESS GAS:	1250.000		4.082	135.121	91.496	174.73	5.25			
3	N2(g)	1250.000		3.465	97.066	77.663	135.87	135.87	39.212	39.212	28.013
4	O2(g)	1250.000		0.046	1.477	1.035	1.91	1.91	41.458	41.458	31.999
5	SO2(g)	1250.000		0.571	36.578	12.798	36.95	-132.53	64.709	-232.104	64.059
6	SLAG:	1300.000		0.283	56.738	0.013	64.75	-274.64			
7	*2FeO*SiO2(l)	1300.000		0.215	43.812	0.010	50.05	-248.03	232.782	-1153.638	203.777
8	Fe2O4(l)	1300.000		0.037	8.490	0.002	10.75	-26.52	293.250	-723.294	231.539
9	Cu2O(l)	1300.000		0.031	4.436	0.001	3.95	-0.09	127.390	-2.831	143.091
10	WHITE METAL:	1250.000		0.469	74.642	0.013	51.51	19.58			
11	Cu2S(l)	1250.000		0.469	74.642	0.013	51.51	19.58	109.837	41.739	159.152
12	METAL:	1250.000		0.000	0.000	0.000	0.00	0.00			
13	Cu(l)	1250.000		0.000	0.000	0.000	0.00	0.00	40.234	48.262	63.546
14	HEAT LOSSES:	1250.000		0.000	0.000	0.000	0.00	0.00			

Fig. 4. The OUT1 sheet of the Heat Balance module. The copper output has been linked with the copper input with a formula and defined name: InCu.

11.5. Elemental Compositions

The elemental compositions of species groups may be calculated using the **Stream Compositions** selection in the **Calculate** menu, see **Fig. 5**. This procedure calculates the elemental compositions of each group, creates new In1-% and Out1-% sheets and prints results on these new sheets in mol% and wt% units.

Note that a procedure to convert elemental analysis back to species analysis is not yet available in the Heat Balance module. A general solution to this kind of problem is quite difficult and in many cases impossible. However, a custom-made solution for an individual case is possible with a little effort and normal Excel-type formulae:

1. Create a new sheet using the **Sheet** selection in the **Insert** menu, see **Fig. 5**.
2. Rename the new sheet by double clicking the tab, for example to “**Compositions**”. Please note that you can use also the Input-% sheet as the starting point when you rename it.
3. Type the elemental and species compositions in the new sheet.
4. Note that you can insert Formula Weights in this new sheet by selecting the chemical formula cells and then selecting **Mol Weight** from the **Insert** menu.
5. Create Excel-type formulae, which convert the elemental analysis of a group to mole amounts of species using formula weights of the elements and species.
6. Type the formulae in the kmol columns of the IN1 sheet, which refer to species amounts in the Compositions sheet.

Element	IN	OUT	Balance	Amount kmol	Amount kg	Content mol-%	Content wt-%
PROCESS GAS:							
N	1250.000	6.930	1243.070	97.066	79.333	71.837	
O		1.234	1.234	19.749	14.130	14.615	
S		0.571	0.571	18.306	6.537	13.548	
SLAG:							
Cu	1300.000	1.855	1298.145	56.738	100.00	100.00	
Fe		0.062	0.062	3.940	3.343	6.944	
O		0.540	0.540	30.157	29.116	53.152	
Si		1.038	1.038	16.602	55.949	29.261	
		0.215	0.215	6.038	11.592	10.643	
WHITE METAL:							
Cu	1250.000	1.407	1248.593	74.642	100.00	100.00	
S		0.938	0.938	59.606	66.667	79.856	
		0.469	0.469	15.036	33.333	20.144	
METAL:							
	1250.000	0.000	1250.000	0.000	0.00	0.00	

Fig. 5. The Out1-% sheet of the Heat Balance module. This sheet shows the elemental compositions of the phases, after the Stream Compositions option has been selected from the Calculate menu.

11.6. Additional Sheets

The Heat Balance workbook consists at least of the IN1, OUT1 and BALANCE sheets. The user may, however, add more sheets to a workbook. These additional sheets may be used, for example, to convert the elemental compositions of raw materials to amounts of species, which are needed in the IN1 sheet. These sheets can also be used to collect the main results from the OUT1 sheet in a summary table. Avoid using the reserved names IN1, OUT1, BALANCE and Target as sheet names.

To add sheets, select **Insert Sheet** from the menu. This will add one sheet in the selected location. To rename this new sheet, double click the Tab at the bottom of the form. You can also import Excel sheets by selecting **Insert Excel Sheet** from the menu. This selection allows you first to select the file and then the sheet which you want to insert into the active Heat Balance workbook.

The example in **Fig. 6** shows a FEED sheet, which is used to specify the raw material amounts in the IN1 sheet. The user can give the compositions and amounts in column C, and this data will then be used to calculate the amounts of species in column F. The material amounts in IN1 sheet are given using relevant cell references to column F in the FEED sheet. This example can be found in your HSC8\Balance directory under the name CUCONV2.bal8. The user can construct the layout of the additional sheets freely.

The “Red Font Shield” property is a useful way of preventing accidental modification of the data in the cells. If this property is set using menu selection **Format, Red Font Shield** then only cells with red font can be edited. However, it is recommended to save the work regularly using different names, for example, test1.bal8, test2.bal8, test3.bal8, etc. in order to recover the original situation after harmful modifications.

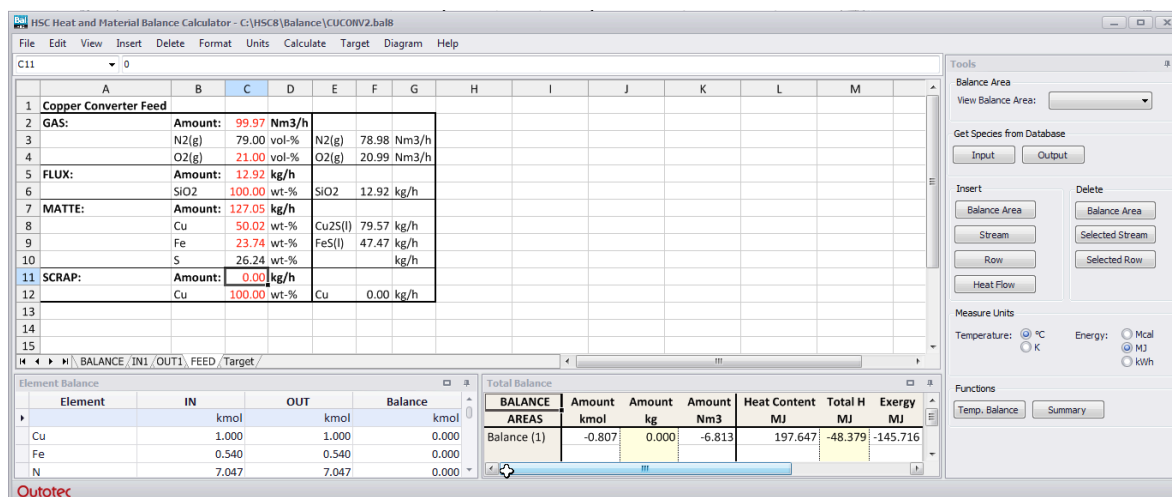


Fig. 6. Additional sheets can be added to the Heat Balance workbook.

11.7. Target Dialog

The user can iterate manually, for example, the fuel amount which is needed to achieve zero heat balance by changing the fuel amount until the heat balance is zero. The Target sheet offers a faster automatic way to carry out these kinds of iterations. The following instructions will explain this procedure in more detail:

1. Select **Target Dialog** from the menu. This will also automatically create a Target sheet, which is similar to previous HSC versions.
2. Select one cell in row 4 in the **Target dialog** if not already selected.
3. Select one cell which will be used as the first variable and select **Set variable cell**. This will add the cell reference of this variable to the Target dialog in column B. *You can also type the cell references manually* in the Target dialog. Note: Please use only Stream temperature cells as variables for the temperature iterations, i.e. do not use species temperature cells.
4. Select one cell which will be used as the first variable and select **Set target cell**. This will add the cell reference of this variable to the Target dialog in column B.
5. Repeat steps 3 and 4 if you want to add more variables and targets.
6. Set valid **Min** and **Max** limits in columns D and E as well as the **Target Value** in column H. You may also type names in columns A and F.
7. Usually it is also necessary to give estimated initial Test Values in column C for the automatic iterations. Iteration ends when the target value (col H) or iteration number (col I) is reached. Accuracy can be improved by increasing the number of decimals used in columns G and H with the **Format Number** selection.
8. Select the rows (> 3) on the Target sheet which you want to iterate and press **Iterate selected rows** or **F8**. If all rows need to be iterated, simply press **Iterate All**.

In the following example, shown in **Fig. 7**, you can select for example row 4 and press **F8**. This will evaluate the copper scrap amount which is needed to maintain the heat balance in the given conditions. Row 5 can be used to iterate the iron content of the matte in the same conditions and row 6 to achieve a given FeS amount.

Important note: Please use only Stream temperature cells as variables for the temperature iterations, i.e. do not use species temperature cells.

Target Dialog

File Edit Insert Delete Iterate

A1 Target Calculation Sheet (Goal seek)

	A	B	C	D	E	F	G	H	I
1	Target Calculation Sheet (Goal seek)								
2	Variable					Target			Iteration
3	Name	Cell Ref.	Test value	Min	Max	Name	Cell Ref.	Value	Max
4	SCRAP	0.00	20.00	0.00	100.00	HEAT BAL	-48.38	0.00	10
5	Fe wt-%	23.74	23.74	0.00	50.00	HEAT BAL	-48.38	0.00	10
6	Fe wt-%	23.74	20.91	0.00	50.00	Fe Amount	0.540	0.540	10
7									10
8									10
9									10
10									10
11									10
12									10
13									10
14									10
15									10
16									10

Target

Ins Row Del Row Set variable cell Set target cell Set goal value Iterate Selected Rows

Exit Iterate All

Fig. 7. The Target dialog specifies the variables and target cell references.

11.8. Graphics

Occasionally, it is useful to see the results of a heat balance calculation, for example, in graphical format. This can be carried out manually by making step-by-step changes to one variable cell and collecting data from cells of interest, for example, in an Excel sheet. Sometimes further calculations may be required after every step, which can be specified using the Diagram Dialog. The step-by-step procedure is as follows:

1. Select **Diagram/Diagram Dialog** from the menu.
2. Select the variable cell and press **Set X-cell** from the dialog. Select, for example, cell C11, see **Fig. 6**.
3. Select a cell for the y-axis and press **Set Y-cell** from the dialog. Select, for example, the Heat Balance cell at the bottom right of the form. You may repeat this step and collect several cells whose values will be drawn in the diagram.
4. If other calculations are required between every step, press **Target iteration** and the Target sheet will automatically open. Select the calculation rows that should be iterated before the Y-row and press **Set Target rows** from the menu. The row data will now be transferred to the Diagram dialog into columns 4, 5, etc.
5. Fill the Diagram Settings as shown in **Fig. 8**. You must specify the MIN, MAX, and STEP values for the X-axis. You can also specify the cell references, labels and units manually in this form.
6. Press **Diagram** to create the tabular data for the diagram and **Diagram** once again to see the final diagram, **Fig. 8**.
7. The diagram can be modified, copied, and printed in the same manner as other diagrams in HSC Chemistry.
8. **Show/Toolbar** shows the drawing menu and **Show/Object Editor** shows the object editor, which lets you specify the objects manually.
9. To return to the Heat Balance module, press **Exit** at the bottom left corner of the diagram form.

In the diagram shown in **Fig. 8**, you can see that roughly 64 kg/h of scrap is needed to adjust the heat balance to zero. Note that the units in the diagram are kg/h and kW.

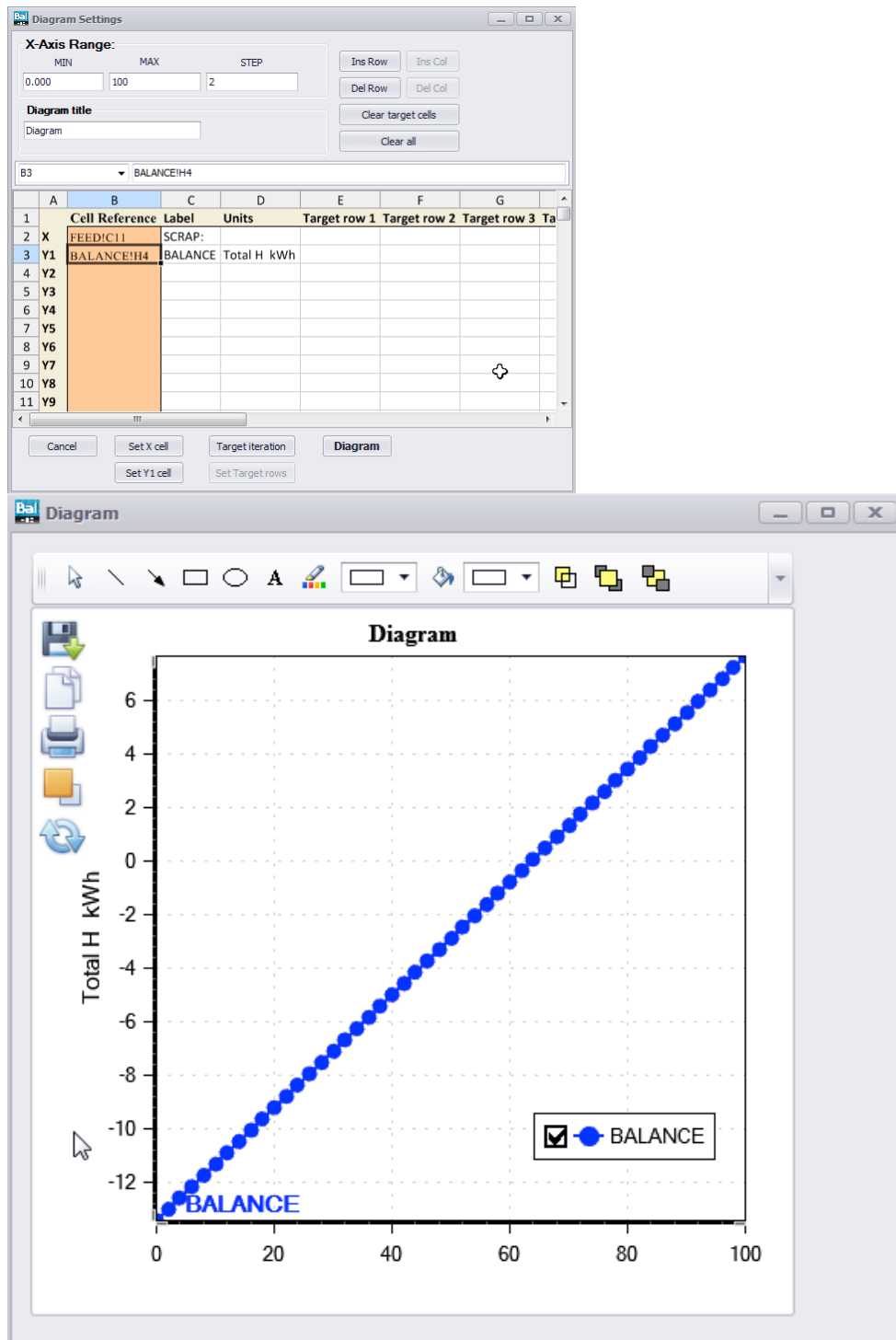


Fig. 8. Simple heat balance diagram.

In the following diagram (**Fig. 9**), the heat balance is automatically calculated before each step, which is indicated by the number “4” in the **Target row 1** column. This is done by pressing the **Target iteration** button, selecting row 4 on the Target sheet and clicking the **Set Target rows** button. The x-axis now gives the Fe wt-% and the y-axis the cooling scrap required. The diagram may then be interpreted as the quantity of cooling scrap required to make the heat balance zero, when the Fe wt-% varies from 20% to 25%.

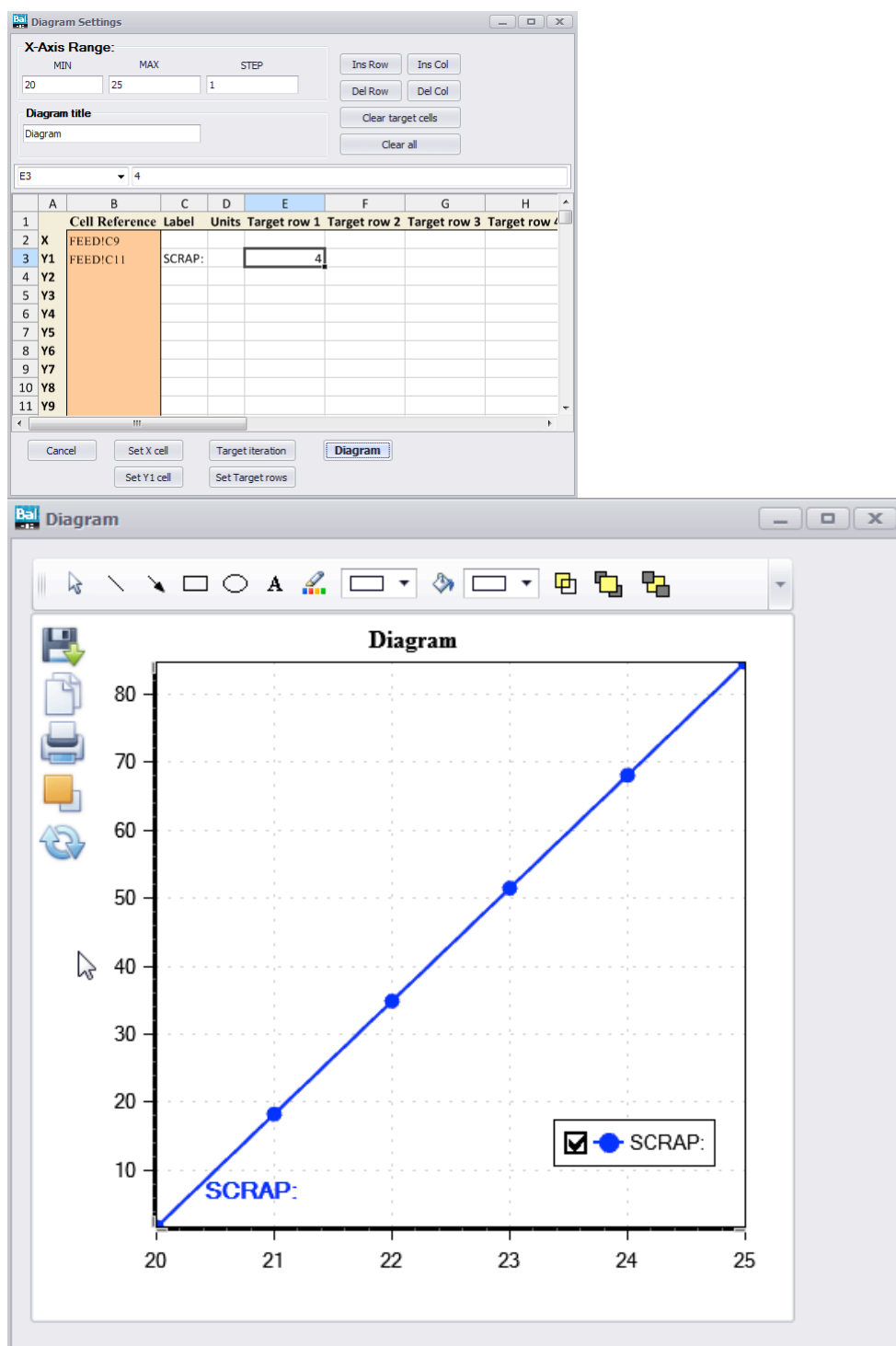


Fig. 9. Diagram where the heat balance is automatically iterated to zero before every calculation step.

11.9. Multiple Balance Areas

Since most processes consist of multiple balance areas, the Balance module enables the user to create multiple balance areas. A balance area consists of an INx and an OUTx sheet, where x denotes the number of the balance area. These can then be connected to each other, creating a realistic simulation of a process. The example file **FSF_process.bal8** contains a highly simplified multibalance model of the Outotec Flash Smelting Furnace process.

A new balance area is created by selecting either **Insert/Balance Area** from the tools sheet. This will insert a pair of INx and OUTx sheets in the corresponding position. It is easy to delete a balance area by selecting **Delete/Balance Area**. However, deleting a single sheet of a balance area, for example in an INx sheet, is not possible. The balances are all automatically collected into the **BALANCE** sheet so please do not modify this sheet.

The screenshot shows the HSC 8 Heat and Material Balance Calculator interface. The main window displays a worksheet with 5 balance areas (IN1 to IN5) and a summary table at the bottom. The summary table is titled 'Total Balance' and lists the following data:

Element	IN	OUT	Balance
Al	1.348	1.348	0.000
Ca	0.674	0.674	0.000
Cu	4.446	4.446	0.000

The summary table also includes columns for 'Amount kmol', 'Amount kg', 'Amount Nm3', 'Heat Content kWh', 'Total H kWh', and 'Exergy kWh'. The 'Amount kmol' column shows values of -4.445, 0.000, and -35.320 for Balance (1), Balance (2), and Balance (3) respectively. The 'Amount kg' column shows values of 0.000, 0.000, and -35.320 for Balance (1), Balance (2), and Balance (3) respectively. The 'Amount Nm3' column shows values of 652.150, 413.465, and 4.982 for Balance (1), Balance (2), and Balance (3) respectively. The 'Heat Content kWh' column shows values of 8.18, 489.57, and 69.33 for Balance (1), Balance (2), and Balance (3) respectively. The 'Total H kWh' column shows values of -1465.31, -1461.51, and -536.70 for Balance (1), Balance (2), and Balance (3) respectively. The 'Exergy kWh' column shows values of 4.334, 306.685, and 22.815 for Balance (1), Balance (2), and Balance (3) respectively.

Fig. 10. A **BALANCE** sheet where the worksheet consists of 5 balance areas.

It is recommended to carry out the linking of balance areas with each other after each individual balance area is operating properly. Linking may be achieved either manually with formulae or automatically with the **Copy - Paste Stream** combination. Simply place the cursor on a stream row in an OUTx sheet, or on a row that belongs to a stream, and select **Edit/Copy**. Then place the cursor on a row in an INx sheet and select **Edit/Paste Stream**. The stream will now be copied here so that the first row of the stream is in the cursor position. The **kmol** column of the pasted stream will consist of links (formulae) to the copied stream, so that the material amounts of the streams will remain equal. The other cells are directly copied as values. If the stream temperature cell in the copied stream is a formula then it will not be copied. In this case it is up to the user to decide how the stream temperature for the pasted stream should be calculated.

It is also possible to create *return streams*, i.e. streams that return to a previous part of the process, thus creating loops in the process. When pasting a stream into an already linked part, a *circular reference* might occur. This is the case when links eventually refer back to each other, i.e. iterations are needed to calculate the worksheet. Automatic iterations may be done by selecting **Format/Options** from the menu and highlighting the **Iteration** checkbox under the **Calculation** tab. Please be careful when changing the inputs of a worksheet consisting of circular references. For example, if a cell, which is part of a circular reference, shows the message **#VALUE!**, it will not be recovered unless the links in the

cells are changed thus breaking the circular reference. Therefore, it is recommended to save the worksheet regularly using different names (Test1, Test2, etc.).

	A	B	C	D	E	F	G	H	I	J	K
	INPUT SPECIES (1)	Temper.	Pressure	Amount	Amount	Amount	Heat Content	Total H	Heat Cont	Tot H	MW
	Formula	°C	bar	kmol	kg	Nm³	kWh	kWh	kWh / kmol	kWh / kmol	
1	Concentrate	25.000		5.589	1000.000	0.255	0.00	-922.89			
2	CuFeS2	25.000		4.091	750.800	0.179	0.00	-216.35	0.000	-52.881	183.513
3	FeS	25.000		0.669	58.800	0.012	0.00	-18.58	0.000	-27.777	87.907
4	FeS2	25.000		0.253	30.400	0.006	0.00	-12.55	0.000	-49.511	119.967
5	CaO*Al2O3*2SiO2	25.000		0.575	160.000	0.058	0.00	-675.41	0.000	-1174.416	278.209
6	Flux	25.000		1.573	112.000	0.042	0.00	-462.98			
7	SiO2	25.000		1.486	89.264	0.034	0.00	-375.89	0.000	-253.016	60.084
8	*2FeO*SiO2	25.000		0.020	4.032	0.001	0.00	-8.13	0.000	-410.864	203.777
9	CaO*Al2O3*2SiO2	25.000		0.067	18.704	0.007	0.00	-78.96	0.000	-1174.416	278.209
10	Air (oxygen enriched)	25.000		23.839	724.823	534.323	0.00	0.00			
11	O2(g)	25.000		14.304	457.696	320.594	0.00	0.00	0.000	0.000	31.999
12	N2(g)	25.000		9.536	267.127	213.729	0.00	0.00	0.000	0.000	28.013
13	Flue dust (Boiler return)	350.000		0.160	29.800	0.006	2.06	-40.06			
14	Cu2O	350.000		0.089	12.723	0.002	0.56	-3.61	6.248	-40.590	143.091
15	Fe3O4(l)	350.000		0.049	11.370	0.002	1.02	-12.85	20.764	-261.610	231.539
16	SiO2	350.000		0.001	0.082	0.000	0.01	-0.34	5.112	-247.903	60.084
17	CaO*Al2O3*2SiO2	350.000		0.020	5.625	0.002	0.48	-23.27	23.660	-1150.757	278.209
18	Flue dust (ESP return)	305.021		0.080	14.900	0.003	0.88	-20.18			
19	Cu2O	305.021		0.044	6.362	0.001	0.24	-1.85	5.332	-41.506	143.091
20	Fe3O4(l)	305.021		0.025	5.685	0.001	0.44	-6.49	17.890	-264.483	231.539
21	SiO2	305.021		0.001	0.041	0.000	0.00	-0.17	4.309	-248.707	60.084
22	CaO*Al2O3*2SiO2	305.021		0.010	2.812	0.001	0.20	-11.67	20.055	-1154.362	278.209
23	Flue dust (Conv. 1 return)	1260.000		0.095	12.099	0.003	4.01	-19.17			
24	Cu2O	1260.000		0.017	2.418	0.000	0.77	-0.02	45.449	-1.389	143.091
25	Fe3O4	1260.000		0.028	6.402	0.001	1.95	-6.62	70.555	-239.306	231.539
26	SiO2	1260.000		0.049	2.932	0.001	1.16	-11.19	23.764	-229.252	60.084
27	CaO*Al2O3*2SiO2	1260.000		0.001	0.351	0.000	0.13	-1.35	106.602	-1067.814	278.209
28	Flue dust (Conv. 2 return)	1260.000		0.027	3.870	0.001	1.23	-0.04			
29	Cu2O	1260.000		0.027	3.870	0.001	1.23	-0.04	45.449	-1.389	143.091
30											

Element	IN	OUT	Balance
	kmol	kmol	kmol
Al	1.348	1.348	0.000
Ca	0.674	0.674	0.000
Cu	4.446	4.446	0.000

Fig. 11. The IN1 sheet (Flash Furnace) of the FSF_process.bal8 example. The stream **Flue dust** is a return stream from the boiler (**Copy/Paste stream**), thus creating *circular references* in the worksheet.

Automatically updated defined names (input and output kmol amounts) vary according to the balance area. For example, InAl, InC, OutFe for the first balance area will become InAl2, InC2, OutFe2 for the second etc. Note that the defined names of the first balance area do not have index numbers.

A	B	C	D	E	F	G	H	I	J	K
OUTPUT SPECIES (2)	Temper.	Pressure	Amount	Amount	Amount	Heat Content	Total H	Heat Cont	Tot H	MW
Formula	°C	bar	kmol	kg	Nm³	kWh	kWh	kWh / kmol	kWh / kmol	
1 Slag	1300.000		1.204	255.673	0.058	105.98	-373.38			
2 *2FeO*SiO2	1300.000		0.843	171.848	0.040	76.24	-270.24	90.409	-320.455	203.777
4 Fe3O4(l)	1300.000		0.304	70.422	0.014	24.78	-61.11	81.458	-200.915	231.539
5 Cu2O(l)	1300.000		0.017	2.415	0.000	0.60	-0.01	35.386	-0.786	143.091
6 CaO*Al2O3*2SiO2	1300.000		0.039	10.989	0.004	4.37	-42.02	110.600	-1063.816	278.209
7 White metal	1260.000		0.512	81.465	0.015	17.54	5.70			
8 Cu2S	1260.000		0.512	81.465	0.015	17.54	5.70	34.274	11.135	159.152
9 Flue dust	1260.000		0.095	12.099	0.003	4.01	-19.17			
10 Cu2O	1260.000		0.017	2.415	0.000	0.77	-0.02	45.449	-1.389	143.091
11 Fe3O4	1260.000		0.028	6.402	0.001	1.95	-6.62	70.555	-239.306	231.539
12 SiO2	1260.000		0.049	2.932	0.001	1.16	-11.19	23.764	-229.252	60.084
13 CaO*Al2O3*2SiO2	1260.000		0.001	0.351	0.000	0.13	-1.35	106.602	-1067.814	278.209
14 Flue gas	1260.000		29.932	997.042	670.889	358.02	127.92			
15 SO2(g)	1260.000		2.791	178.779	62.553	50.62	-179.48	18.137	-64.312	64.059
16 N2(g)	1260.000		12.603	353.051	282.477	138.50	138.50	10.989	10.989	28.013
17 O2(g)	1260.000		14.538	465.212	325.858	168.90	168.90	11.618	11.618	31.999
18 Flue dust (Conv. 1 return)	1260.000		0.095	12.099	0.003	4.01	-19.17			
19 Cu2O	1260.000		0.017	2.415	0.000	0.77	-0.02	45.449	-1.389	143.091
20 Fe3O4	1260.000		0.028	6.402	0.001	1.95	-6.62	70.555	-239.306	231.539
21 SiO2	1260.000		0.049	2.932	0.001	1.16	-11.19	23.764	-229.252	60.084
22 CaO*Al2O3*2SiO2	1260.000		0.001	0.351	0.000	0.13	-1.35	106.602	-1067.814	278.209
23 Heat loss (Converter I):							10.00			

Element	IN	OUT	Balance
	kmol	kmol	kmol
Al	1.348	1.348	0.000
Ca	0.674	0.674	0.000
Cu	4.446	4.446	0.000

AREAS	Amount	Amount	Amount	Heat Content	Total H	Exergy
	kmol	kg	Nm³	kWh	kWh	kWh
Balance (1)	-4.445	0.000	-56.124	652.150	3.808	-324.663
Balance (2)	-3.956	0.000	-35.320	413.465	4.982	-118.353

Fig. 12. The OUT2 sheet (Converter I), gives the output from the first part of the converter. The formula `=InCa2*Analysis!L29/100` in cell C5 means that the total Ca is distributed as the percentage given in cell L29 on the Analysis sheet.

Drawing Flowsheets (Flowcharts)

Additional sheets may be used to collect, for example, all the necessary input for the process into one sheet. They may also be used to collect calculated process parameters, for example the amount of Cu in a stream. **Fig. 13** shows the process layout for the Flash Smelting Furnace process.

The "Insert, Graphical Object, ..." selection offers the possibility to draw lines, rectangles, etc. on the additional sheets. However, it is recommended to draw flowsheets using the "Format, Border, ..." and "Format, Pattern, ..." selections because these properties are more compatible with Excel. Arrows may be drawn using the "Insert, Graphical Object, Arrow" selection.

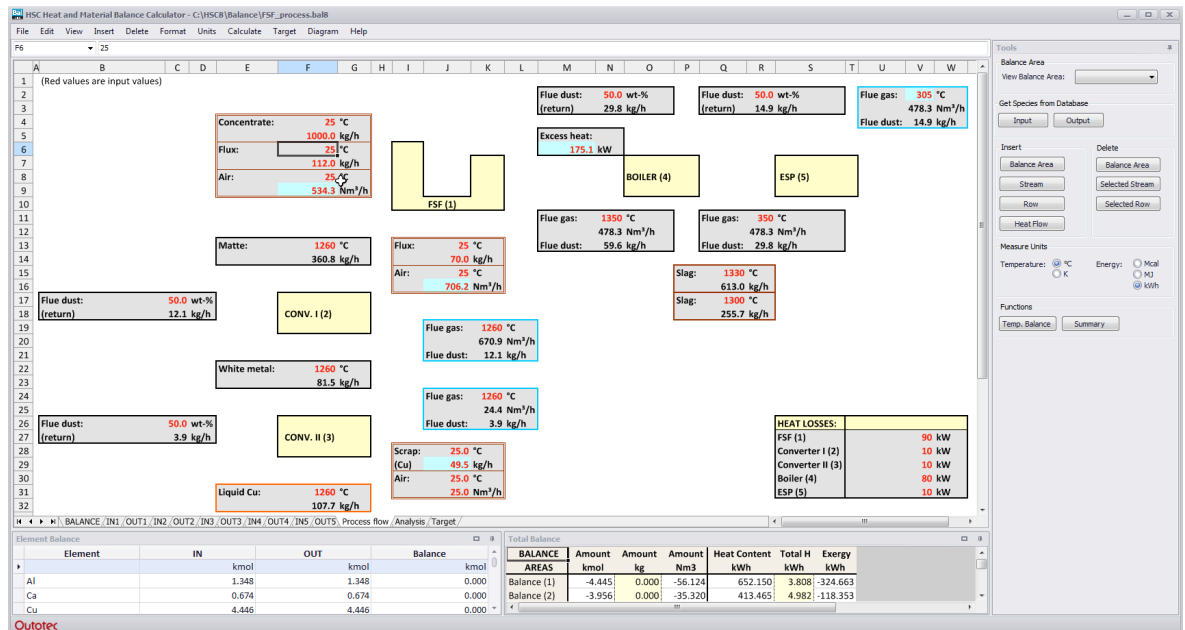


Fig. 13. Process layout and input sheet for the Flash Smelting Furnace process.

Fig. 14 provides a more detailed analysis of the process. The model is constructed so that the inputs are given as species analysis and the outputs are calculated. The elemental distributions are also inputs, in other words the user defines the wt-% for the elemental distributions into the given species and streams. This is achieved by using the automatically defined names, for example InCa and InO2, thus always keeping the elemental balance at zero. The model may then be used to balance the heat balances of the process, which enables the user to calculate one unknown parameter per balance area. The unknown parameters calculated in the FSF_process.bal8 example are indicated by a light blue cell background. The calculated parameters may be changed using the **Target Dialog** option, which is described in further detail in Section 11.7. Target Dialog.

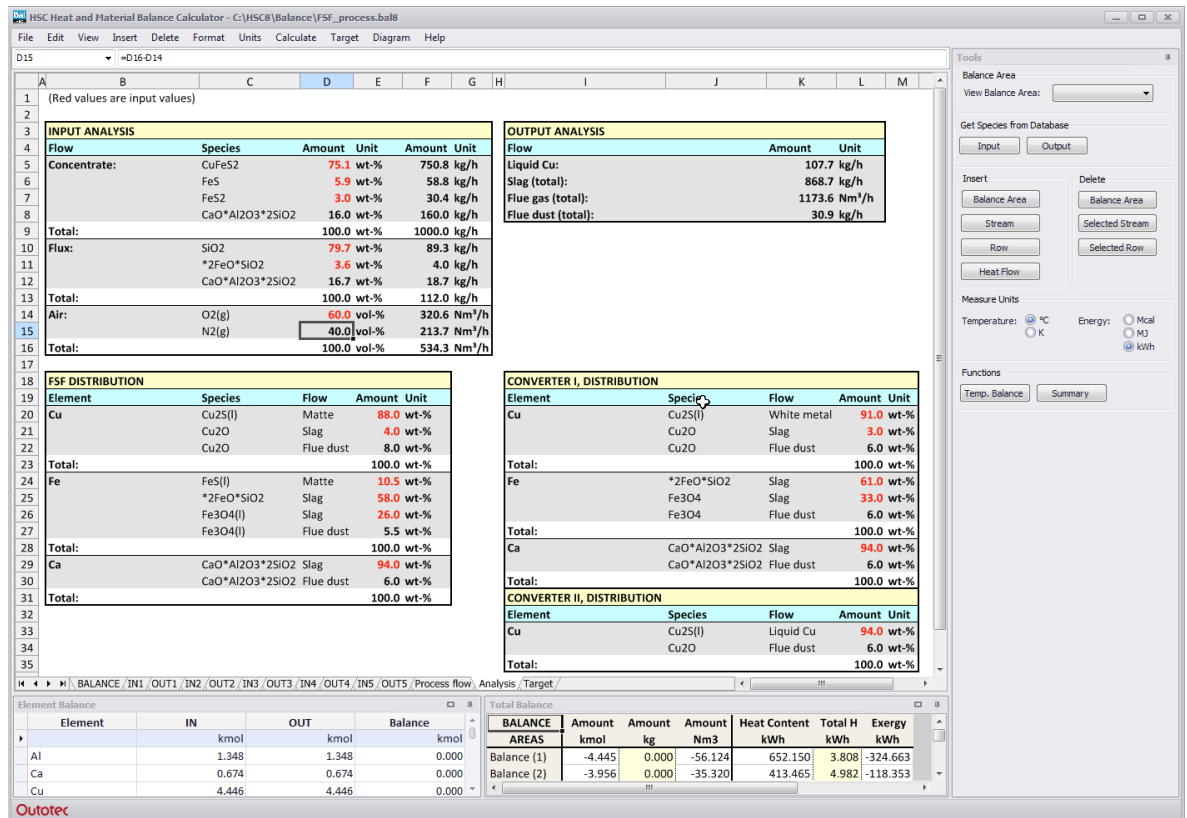


Fig. 14. Detailed analysis of the input and output streams and the elemental distributions into different species. The distributions are given in wt-% (weight percentage).

11.10. General Considerations

In the **Heat Balance** module it is possible to use the new add-in functions provided by HSC 8.0. The functions should be enabled automatically. Sometimes it is necessary to browse the location of the add-in file manually. A more detailed description of the functions available may be found in Chapter 30. Excel Add-Ins. It is, however, not recommended to use add-in functions for very large worksheets, since a complete recalculation of the worksheet is necessary each time a change is made in the worksheet. This is the case *only* when using add-in functions.

Please do not use temperature formulae that are linked to other temperature values *within a stream*, instead link them to the *stream* temperature cell or any cell in a user sheet. Otherwise, the temperatures will be updated only after the next change. Please also note that a change in the temperature value is required for the whole stream to be updated accordingly.

Simple graphical objects may be inserted by selecting **Insert/Graphical Object** from the menu. The shapes are: Line, Rectangle, Oval, Arc, and Polygon. After inserting, the objects may be modified by first selecting the object and then selecting **Format/Object** from the menu.

The **Heat Content** column (= specific heat) is used to describe the energy which may be released when the compound is cooled down from the given temperature to 298.15 K. In other words, it contains latent heat (= enthalpies of the possible phase transformations) as well as specific heat. The enthalpies given in the **Total H** column contain the values of the Heat Content column as well as the heat of formation reactions. These values are used to calculate heat balances.

In **molten mixtures** such as oxide slags, substances can exist in liquid state at lower temperatures than their melting points. In these cases, it is possible to use an (l)-suffix at the end of the formulae, see **Fig. 1**. This will force HSC to use the data of the liquid state for species with an (l)-suffix.

The “**Red Font Shield**” property is sometimes useful if you want to prevent accidental changes to cells. You can activate this property by selecting **Format Red Font Shield** from the menu. After this selection you can edit only those cells which contain red font.

If you have carried out a laboratory- or industrial-scale experiment or process calculations you usually know:

1. The raw (input) materials and their amounts and temperatures.
2. The product (output) materials and their amounts, temperatures and analysis.
3. The input heat and heat losses can first be estimated as zero, if not available.

In order to calculate a heat balance, you must first convert the (elemental) chemical analysis of the raw materials and the products into input and output substances (species). Sometimes this step is the most difficult, so you may choose to carry out this procedure using the HSC Species Converter module, see Chapter 22. Species Converter. When this is completed, simply type the input substances (species) into the IN1 Sheet and the output substances into the OUT1 sheet. Immediately after that you will see the heat and material balance on the bottom line. You can also test the procedure described in Section 11.5.

It is important to check the element balance by selecting **Calculate/Element Balance**, in order to avoid incorrect material and heat balances. This can also be used to check the validity of the chemical analyses and the other amount measurements of the experiment if the user input is based on this data.

When creating a multiple balance area model, selecting **Calculate/Total Balance** shows an overview of all balance areas in one window. This is useful for a quick check where the material and/or heat balance are not zero. It also shows the total (or net) material and heat balance for all balance areas. It is then easy to see which balance areas produce heat, which require heat, and indications of how the heat could be transferred within the process.

On the basis of the final results, conclusions can be made as to whether extra energy is needed or increased insulation is required or if the reactor needs cooling on a large scale. The heat losses may also be determined using the HeatLoss module. Combining the two modules provides a powerful way of calculating processes.

It is important to note that this is a real heat balance for engineering purposes, which also takes into account the kinetic aspects if the user input is based on real experimental data. The heat balance, which can be obtained from the equilibrium calculations, is theoretical in this respect. It is valid only if the equilibrium is reached in the real process.

11.11. Heat Balance Examples

See the examples provided by the HSC package by selecting **File/Open** from the menu, see **Fig. 1**, and selecting some of the ready-made files in the directory for editing. HSC 8.0 can read the old HSC 2.0 Heat Balance text files, but it cannot save them in the old format. The new HSC 8.0 Heat Balance files save all the sheets and formats, not only the text data.

1. Preliminary check for a heat balance (CUSMELT.bal8 file)

For some processes based on reaction equations or equilibrium calculations, the heat balance can easily be checked by entering the assumed input and output substances as well as their temperatures and amounts, see example CUCONV.bal8 and CUSMELT.bal8, **Fig. 1**.

2. Adiabatic temperature of a flame (BUTANE.bal8 file)

In an adiabatic process, heat losses from and heat input to the system are zero, i.e. there is no heat exchange with the surroundings through the system boundaries. Therefore, the adiabatic temperature equals the highest attainable temperature from a flame or a chemical reaction. By typing the raw materials into the IN1 sheet and the products into the OUT1 sheet, it is possible to see the adiabatic temperature by selecting Temperature Balance from the Calculate menu, **Fig. 2**, see example BUTANE.bal8.

3. Dimensioning of an evaporator (H2O.bal8 file)

The evaporator dimensions can be optimized manually by typing the input substances into the IN1 sheet and the desired output substances, amounts and temperatures into the OUT1 sheet. Once these have been entered, you can start to change the amount or temperature of the input vapor (input heat if heated by electricity) manually, in order to find the optimum values. See the example of H2O.bal8.

4. Net and gross heat value of coal, fuel oil and natural gas (Coal1-, Coal2-, FuelOil1-, FuelOil2-, NatGas1.bal8 files)

The **Heat balance** module makes it possible to calculate the Heat Values (Calorific Values) for different fuels. Examples for coal, fuel oil and natural gas are found in the example files. Note that the chemical structures of fuel oil and coal are very complicated. However, heat values based on elemental analysis will usually give sufficiently accurate results for practical applications.

5. Outotec Flash Smelting Furnace process (FSF_process.bal8 file)

This highly simplified process case consists of five balance areas linked together. The balance areas are:

- 1) Flash Smelting Furnace
- 2) Converter I
- 3) Converter II
- 4) Boiler
- 5) ESP

The process input values are provided in the sheets **Process flow** and **Analysis**. By pressing **F8** or by selecting **Iterate All** from the **Target Dialog**, the heat balances are calculated. The values calculated are in the sheet **Process flow** and indicated by a light blue cell background.

6. Iron production process (Iron_process.bal8 file).

The example in this file is a very simplified model of an iron production process consisting of three balance areas:

- 1) Pelletizing
- 2) Coking
- 3) Reduction

The process and its most important parameters are shown in the sheet **Process flow**, with a more detailed analysis available in the sheet **Analysis**. Notice that only the material balances are zero and iterated according to what is set in the **Target sheet** (or **Target dialog**). The heat balances are not iterated and therefore not zero.