

11. HEAT AND MATERIAL BALANCE

	INPUT SPECIES (1) Formula	Temper. °C	Amount kmol	Amount kg	Amount Nm ³	Latent H MJ	Total H MJ
1	GAS:	25.000	4.386	126.537	99.971	0.000	0.000
2	N2(g)	25.000	3.465	97.066	78.980	0.000	0.000
3	O2(g)	25.000	0.921	29.471	20.991	0.000	0.000
4	FLUX:	25.000	0.215	12.918	0.005	0.000	-195.834
5	SiO2	25.000	0.215	12.918	0.005	0.000	-195.834
6	MATTE:	1250.000	1.040	127.046	0.024	96.296	27.347
7	Cu2S(l)	1250.000	0.500	79.576	0.014	54.919	20.869
8	FeS(l)	1250.000	0.540	47.470	0.010	41.377	6.477
9	COOLING SCRAP:	25.000	0.000	0.000	0.000	0.000	0.000
10	Cu	25.000	0.000	0.000	0.000	0.000	0.000
11	EXTRA HEAT:						0.000
12							
13							
14							
15							
16							
17							
			kmol	kg	Nm ³	MJ	MJ
BALANCE (1)			-0.807	0.000	-6.929	209.86	-80.74

Fig. 1. Heat and Material Balance workbook with IN1, OUT1 and BAL 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 IN1, OUT1 and BAL sheets. A pair of IN and OUT sheets is called a *Balance area*, which may be considered equivalent to a control volume. A total number of 127 balance areas may be inserted, to create a multiple balance area workbook. Multiple balance area workbooks are explained in more detail in chapter 10. *Multiple balance areas*. For 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 BAL 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 BAL sheet.

Since the program uses and creates new balance areas according to the name of the sheets, it is extremely important that *the automatically created sheet names, i.e. the BAL, 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 IN1 sheet using normal Excel cell references, for example, for converting elemental analysis of the raw material to amounts of the components.
- use the heat balance calculation results in 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 names 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 and was available already in HSC 2.0. However, the problem with the old version was that the user had to manually maintain the material balance when the input feed changed.
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. Introduce the input substances (raw materials), temperatures and amounts on 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. Introduce the output substances (products), temperatures and amounts on the OUT1 sheet. Type amounts in either kmol, kg or Nm³ as preferred.
3. When feeding additional energy (electricity) to the process, enter this 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. 20. The Database module will convert the color of all “inert” text in the first column to green, if this text is not identified in the database as a substance. Notice that:

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

However, the Balance module will automatically recalculate green text when changing 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.

- 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:

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

Where:

A	=	Outer surface area of the reactor (m ²)
T ₂	=	Surface temperature of the reactor (°C)
T ₁	=	Room temperature (°C)

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

- HSC automatically and immediately updates the heat balance on the bottom line as soon as changes to any input data are made.
- HSC also automatically updates the material amount balances in mol, kg and Nm³ units. Notice 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.
- The element balance can be checked by selecting **Element Balance** from the **Calculate** menu, see Figs. 1 and 2.
- By selecting **Temperature Balance** from the **Calculate** menu it is possible to see the estimated temperature of the products when the heat balance = 0, see Figs. 1 and 3.

	IN1	OUT1	BALANCE
	kmol	kmol	kmol
Cu	1.000	1.000	0.000
Fe	0.540	0.540	0.000
N	6.930	6.930	0.000
O	2.272	2.272	0.000
S	1.040	1.040	0.000
Si	0.215	0.215	0.000
	kg	kg	kg
Cu	63.546	63.546	0.000
Fe	30.157	30.157	0.000
N	97.066	97.066	0.000
O	36.351	36.351	0.000
S	33.342	33.342	0.000
Si	6.038	6.038	0.000

Fig. 2. Element Balance.

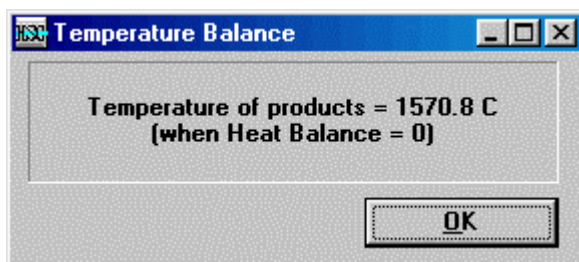


Fig. 3. Temperature of the products (adiabatic process).

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 **Units** menu.
13. Energy units can be changed by selecting **Mcal**, **MJ** or **kWh** from the **Units** menu.
14. If a paper copy is needed, select **Print** from the **File** menu. This option will copy all the data on 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 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 will open the Pressure and Temperature calculator, where it is possible to specify the pressure for the species. This is useful when calculating for example steam processes.

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. The **Normal** selection gives a VGA size window, **Full Height** selection uses the whole height of the screen and **Full Width** fills the whole screen.

11.3 Specification of Substance Groups (Streams)

The new HSC Chemistry 5.0 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 the 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 if the species are not divided into streams.*

Examples of “one-phase streams” are, for example:

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

Examples of “multi-phase streams” are, for example:

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, total amount of the stream and the total material and heat balance as well.

An example of the species streams can be seen in Fig. 4. 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.

	OUTPUT SPECIES (1) Formula	Temper. °C	Amount kmol	Amount kg	Amount Nm ³	Latent H MJ	Total H MJ
1	PROCESS GAS:	1250.000	4.082	135.121	93.044	174.772	5.292
2	N2(g)	1250.000	3.465	97.066	78.980	135.910	135.910
3	O2(g)	1250.000	0.046	1.477	1.052	1.913	1.913
4	SO2(g)	1250.000	0.571	36.578	13.012	36.949	-132.531
5	SLAG:	1300.000	0.283	56.738	0.013	79.874	-274.095
6	*2FeO*SiO2(l)	1300.000	0.215	43.812	0.010	65.949	-247.561
7	Fe3O4(l)	1300.000	0.037	8.490	0.002	9.976	-26.446
8	Cu2O(l)	1300.000	0.031	4.436	0.001	3.949	-0.088
9	WHITE METAL:	1250.000	0.469	74.642	0.013	51.514	19.576
10	Cu2S(l)	1250.000	0.469	74.642	0.013	51.514	19.576
11	METAL:	1250.000	0.000	0.000	0.000	0.000	0.000
12	Cu(l)	1250.000	0.000	0.000	0.000	0.000	0.000
13	HEAT LOSSES:						0.000
14							
15							
16							
17							

			kmol	kg	Nm ³	MJ	MJ
Exit	< >	BALANCE (1)	-0.807	0.000	-6.929	209.86	-80.74

Fig. 4. 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 Cu₂S in the cell OUT1!C10 contains 93.8 % of copper input then you may type formula = **0.938*IN1!C7** in cell OUT1!C10, see Fig 5.
2. The Heat balance module automatically calculates 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 automatically iterate the circular references. This is, however, not recommended for very large worksheets.

Within 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 use the formulae also in other columns, but please be very careful. In the other sheets there are no special limitations for the formulae.

Heat and Material Balance - D:\HSC5\Balance\Cuconv1.bal

File Edit View Insert Delete Format Units Calculate Target Diagram Options Help

C10 =0.938*(InCu-C12)/2

	OUTPUT SPECIES (1) Formula	Temper. °C	Amount kmol	Amount kg	Amount Nm ³	Latent H MJ	Total H MJ
1	PROCESS GAS:	1250.000	4.082	135.121	93.044	174.772	5.292
2	N2(g)	1250.000	3.465	97.066	78.980	135.910	135.910
3	O2(g)	1250.000	0.046	1.477	1.052	1.913	1.913
4	SO2(g)	1250.000	0.571	36.578	13.012	36.949	-132.531
5	SLAG:	1300.000	0.283	56.738	0.013	79.874	-274.095
6	*2FeO*SiO2(l)	1300.000	0.215	43.812	0.010	65.949	-247.561
7	Fe3O4(l)	1300.000	0.037	8.490	0.002	9.976	-26.446
8	Cu2O(l)	1300.000	0.031	4.436	0.001	3.949	-0.088
9	WHITE METAL:	1250.000	0.469	74.642	0.013	51.514	19.576
10	Cu2S(l)	1250.000	0.469	74.642	0.013	51.514	19.576
11	METAL:	1250.000	0.000	0.000	0.000	0.000	0.000
12	Cu(l)	1250.000	0.000	0.000	0.000	0.000	0.000
13	HEAT LOSSES:						0.000
14							
15							
16							
17							

Exit BAL IN1 OUT1 kmol kg Nm³ MJ MJ

BALANCE (1) -0.807 0.000 -6.929 209.86 -80.74

Fig. 5. The OUT1 sheet of the Heat Balance module. Copper output has been linked with copper input with a formula and defined name: InCu.

11.5 Elemental Compositions

The elemental compositions of the species groups may be calculated using the **Stream Compositions** selection in the **Calculate** menu, see Fig. 6. 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.

Notice 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. 6.
2. Rename the new sheet by double clicking the tab, for example to “**Compositions**”. Notice that you can use also the Input-% sheet as the starting point as you rename it.
3. Type the elemental and species compositions on the new sheet.
4. Notice 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 formulae in the kmol columns of the IN1 sheet, which refer to species amounts in the Compositions sheet.

Heat and Material Balance - D:\HSC5\Balance\Cuconv1.bal

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C11 0.938

	OUT1 Compositions	Temper. °C	Amount kmol	Amount kg		Content mol-%	Content wt-%
1	PROCESS GAS:	1250.000	8.735	135.121		100.000	100.000
2	N		6.930	97.066		79.333	71.837
3	O		1.234	19.749		14.130	14.615
4	S		0.571	18.306		6.537	13.548
5	SLAG:	1300.000	1.855	56.738		100.000	100.000
6	Cu		0.062	3.940		3.343	6.944
7	Fe		0.540	30.157		29.116	53.152
8	O		1.038	16.602		55.949	29.261
9	Si		0.215	6.038		11.592	10.643
10	WHITE METAL:	1250.000	1.407	74.642		100.000	100.000
11	Cu		0.938	59.606		66.667	79.856
12	S		0.469	15.036		33.333	20.144
13	METAL:	1250.000	0.000	0.000		0.000	0.000
14							
15							
16							
17							
18							

← BAL IN1 OUT1 In1-% Out1-%

Exit	< >	BALANCE (1)	kmol	kg	Nm ²	MJ	MJ
			-0.807	0.000	-6.929	209.86	-80.74

Fig. 6. 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 BAL sheets. The user may, however, add up to 256 sheets to one 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 one summary table. Do not use the reserved names IN1, OUT1, BAL and Target as sheet names.

To add sheets select **Insert Sheet** from the menu. This will add one sheet on the selected location. To rename this new sheet, double click the Tab on 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. 7 shows a FEED sheet, which is used to specify the raw materials amounts to the IN1 sheet. The user may give the compositions and amounts in column C, 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 from your HSC5\Balance directory under the name CUCONV2.BAL. The user can construct the layout of the additional sheets freely.

The “Red Font Shield” property is a useful way to prevent 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.bal, test2.bal, test3.bal, etc. in order to recover the original situation after harmful modifications.

Heat and Material Balance - D:\HSC5\Balance\Cuconv2.bal

File Edit View Insert Delete Format Units Calculate Target Diagram Options Help

C11 0

	A	B	C	D	E	F	G	H
1	Copper Converter Feed							
2	GAS:	Amount:	99.97	Nm ³ /h				
3		N ₂ (g)	79.00	vol-%	N ₂ (g)	78.98	Nm ³ /h	
4		O ₂ (g)	21.00	vol-%	O ₂ (g)	20.99	Nm ³ /h	
5	FLUX:	Amount:	12.92	kg/h				
6		SiO ₂	100.00	wt-%	SiO ₂	12.92	kg/h	
7	MATTE:	Amount:	127.05	kg/h				
8		Cu	50.02	wt-%	Cu ₂ S(l)	79.57	kg/h	
9		Fe	23.74	wt-%	FeS(l)	47.47	kg/h	
10		S	26.24	wt-%			kg/h	
11	SCRAP:	Amount:	0.00	kg/h				
12		Cu	100.00	wt-%	Cu	0.00	kg/h	
13								
14								
15								
16								
17								
18								

← BAL IN1 OUT1 FEED Target →

Exit < > BALANCE (1) kmol kg Nm² MJ MJ

-0.807 0.000 -6.929 209.86 -50.74

Fig. 7. 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 kind 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 on row 4 in the Target dialog if not selected.
3. Select one cell which will be used as a 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, ie. do not use species temperature cells.
4. Select one cell which will be used as 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 should be iterated, simply press **Iterate All**.

In the following example, shown in Fig. 8, 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, ie. do not use species temperature cells.

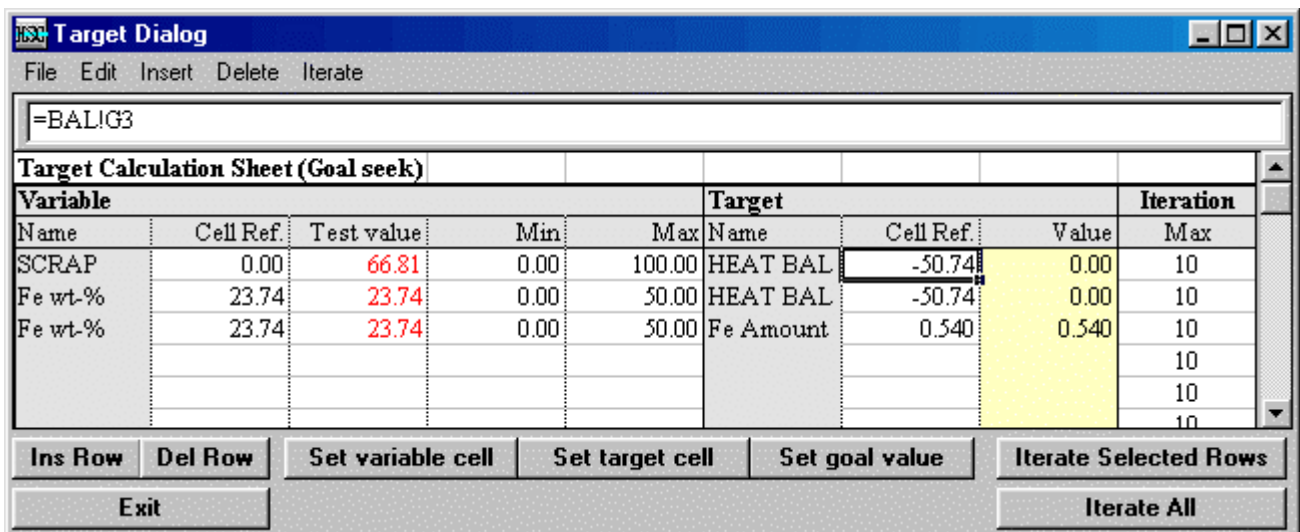


Fig. 8. Target dialog specifies the variables and target cell references.

11.8 Graphics

Occasionally it is useful to see the results, of for example a heat balance calculation, in graphical format. This can be carried out manually by making step by step changes to one variable cell and collecting data from interesting cells, for example, to an Excel sheet. Sometimes further calculations may be required after every step, which can be specified using the Diagram Dialog. Step by step the 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. 7.
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 to 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. 9. 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 9.
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.

From the diagram shown in Fig. 9 you can see that roughly 68 kg/h of scrap is needed to adjust the heat balance to zero. Notice that the units in the diagram are kg/h and kW.

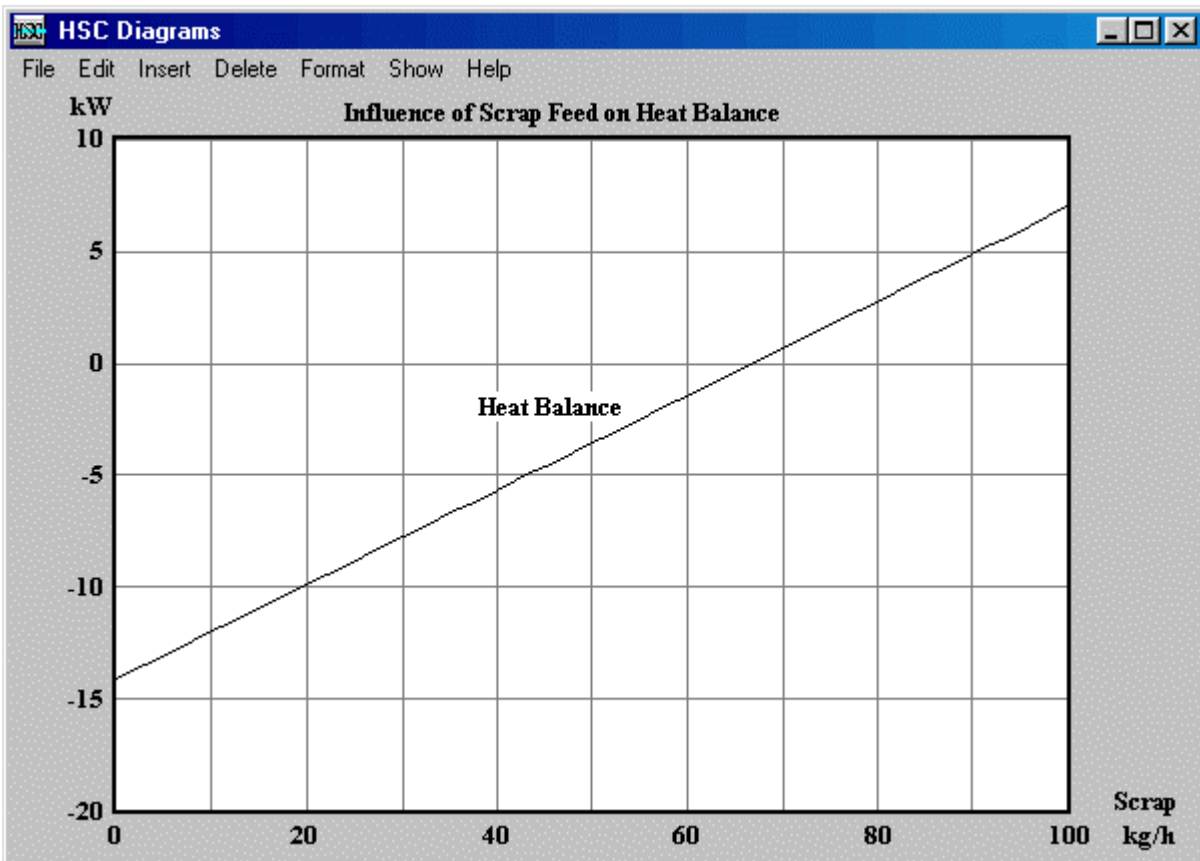
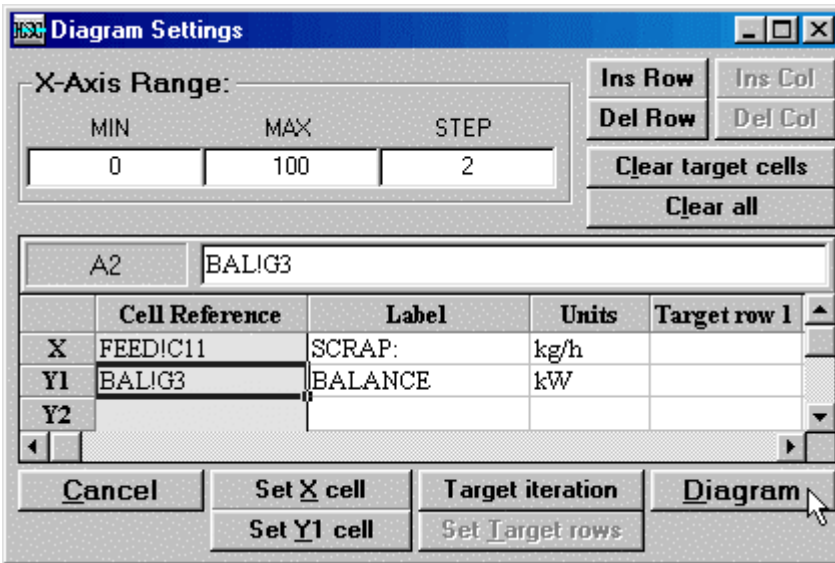


Fig. 9. Simple heat balance diagram.

In the following diagram (Fig. 10) 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%.

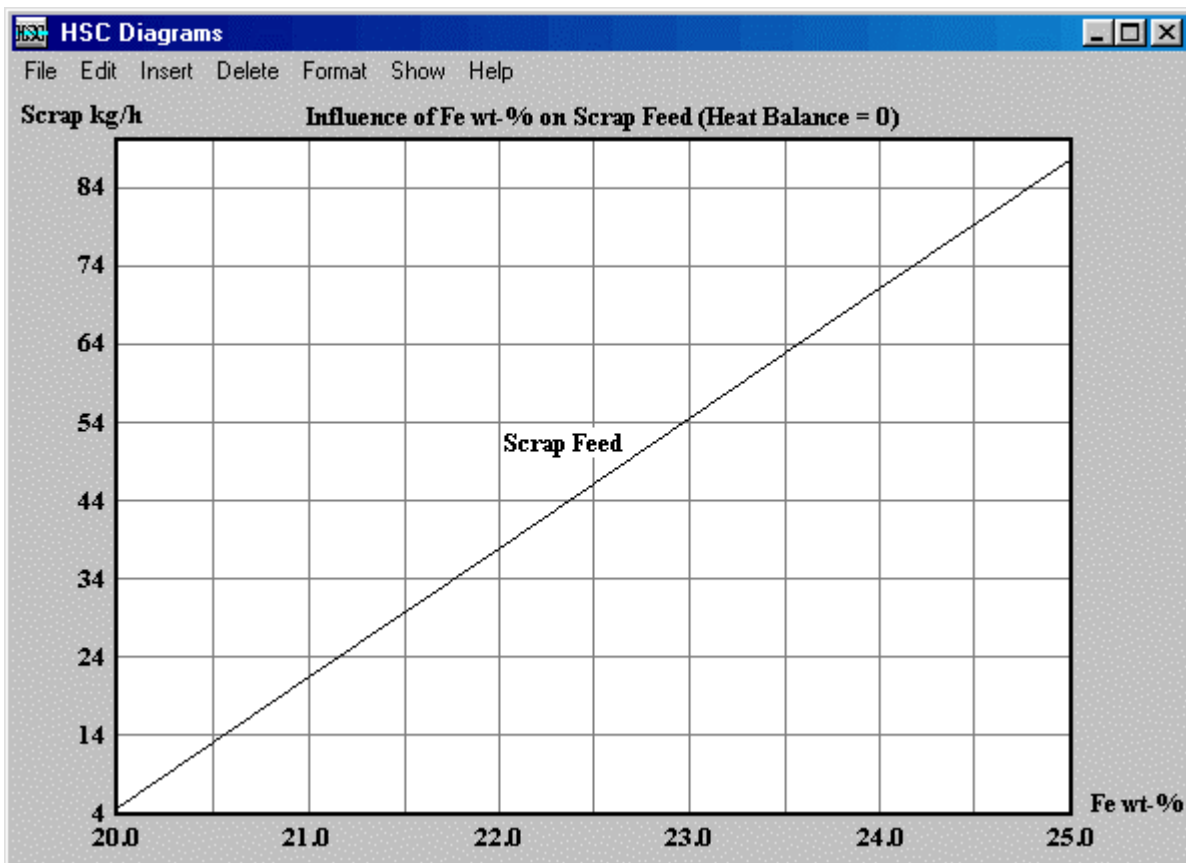
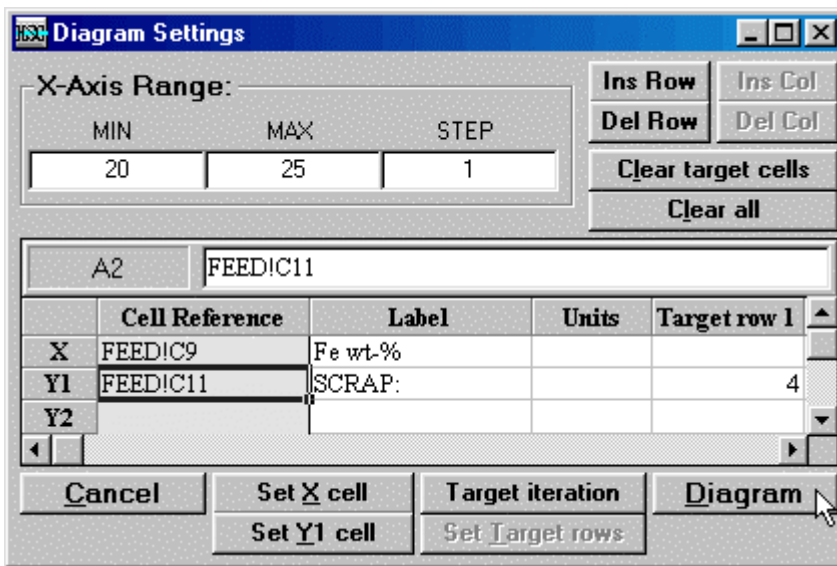


Fig. 10. Diagram where the heat balance is automatically iterated to zero before every calculation step.

11.9 Multiple balance areas

The previous Balance modules up to HSC 4.0 were restricted to one balance area (or control volume) only. Since most processes consist of multiple balance areas, the new Balance module enables the user to create up to 127 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.BAL** contains a highly simplified multibalance model of an Outokumpu Flash Smelting Furnace process.

A new balance area is created by selecting either **Insert/Balance Area to Right** or **Insert/Balance Area to Left** from the menu. This will insert a pair of INx and OUTx sheets to the corresponding position. A balance area may easily be deleted by selecting **Delete/Balance Area**. Deleting a single sheet of a balance area, for example an INx sheet, is not possible. The balances are all automatically collected into the **BAL** sheet so please do not modify this sheet.

	BALANCE	Temper. °C	Amount kmol	Amount kg	Amount Nm ³	Latent H kWh	Total H kWh
1	IN1		30.966	1885.455	534.633	8.09	-1464.91
2	OUT1		26.521	1885.455	477.547	653.75	-1464.91
3	BALANCE		-4.445	0.000	-57.086	645.66	0.00
4							
5	IN2		35.270	1342.469	706.286	76.10	-273.10
6	OUT2		31.314	1342.469	670.365	482.57	-273.10
7	BALANCE		-3.956	0.000	-35.921	406.46	0.00
8							
9	IN3		2.388	164.337	25.020	17.60	6.06
10	OUT3		2.819	164.337	24.396	40.83	6.06
11	BALANCE		0.431	0.000	-0.624	23.23	0.00
12							
13	IN4		21.262	911.638	477.321	325.54	-322.07
14	OUT4		21.262	911.638	477.321	70.41	-322.07
15	BALANCE		0.000	0.000	0.000	-255.13	0.00
16							
17	IN5		21.102	881.838	477.315	68.42	-537.34
18	OUT5		21.102	881.838	477.315	58.42	-537.34
19	BALANCE		0.000	0.000	0.000	-10.00	0.00

Fig. 11. The BAL sheet when the worksheet consists of 5 balance areas.

Linking the balance areas with each other is recommended to carry out after each individual balance areas operate 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 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 formulae 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 recover unless the links in the cells are changed thus breaking the circular reference. Saving the worksheet regularly using different names (Test1, Test2, etc.) is thus always recommended.

Heat and Material Balance - C:\Hsc5\Balance\FSF_process.BAL

File Edit View Insert Delete Format Units Calculate Target Diagram Options Help

C14 =OUT4IC11

	INPUT SPECIES (1) Formula	Temper. °C	Amount kmol	Amount kg	Amount Nm ³	Latent H kWh	Total H kWh
1	Concentrate	25.000	5.589	1000.000	0.255	0.00	-922.73
2	CuFeS2	25.000	4.091	750.800	0.179	0.00	-216.35
3	FeS	25.000	0.669	58.800	0.012	0.00	-18.89
4	FeS2	25.000	0.253	30.400	0.006	0.00	-12.07
5	CaO*A12O3*2SiO2	25.000	0.575	160.000	0.058	0.00	-675.41
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
8	*2FeO*SiO2	25.000	0.020	4.032	0.001	0.00	-8.13
9	CaO*A12O3*2SiO2	25.000	0.067	18.704	0.007	0.00	-78.96
10	Air (oxygen enriched)	25.000	23.443	712.787	534.323	0.00	0.00
11	O2(g)	25.000	14.067	450.114	320.594	0.00	0.00
12	N2(g)	25.000	9.377	262.673	213.729	0.00	0.00
13	Flue dust (Boiler return)	350.000	0.160	29.800	0.006	1.99	-39.86
14	Cu2O	350.000	0.089	12.723	0.002	0.56	-3.66
15	Fe3O4(l)	350.000	0.049	11.370	0.002	0.95	-12.60
16	SiO2	350.000	0.001	0.082	0.000	0.01	-0.34
17	CaO*A12O3*2SiO2	350.000	0.020	5.625	0.002	0.48	-23.27
18	Flue dust (ESP return)	305.021	0.080	14.900	0.003	0.85	-20.08
19	Cu2O	305.021	0.044	6.362	0.001	0.24	-1.87
20	Fe3O4(l)	305.021	0.025	5.685	0.001	0.41	-6.37
21	SiO2	305.021	0.001	0.041	0.000	0.00	-0.17
22	CaO*A12O3*2SiO2	305.021	0.010	2.812	0.001	0.20	-11.67

BAL IN1 OUT1 IN2 OUT2 IN3 OUT3 IN4 OUT4 IN5 OUT5

Exit Stream < > BALANCE (1) kmol kg Nm³ kWh kWh

-4.445 0.000 -57.086 645.66 0.00

Fig. 12. The IN1 sheet (Flash Furnace) of the FSF_process.BAL 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.

	OUTPUT SPECIES (2) Formula	Temper. °C	Amount kmol	Amount kg	Amount Nm ³	Latent H kWh	Total H kWh
1	Slag	1300.000	1.204	255.673	0.058	104.89	-372.70
2	*2FeO*SiO2	1300.000	0.843	171.848	0.040	76.94	-269.73
3	Fe3O4(l)	1300.000	0.304	70.422	0.014	22.99	-60.93
4	Cu2O(l)	1300.000	0.017	2.415	0.000	0.60	-0.01
5	CaO*Al2O3*2SiO2	1300.000	0.039	10.989	0.004	4.37	-42.02
6	White metal	1260.000	0.512	81.465	0.015	17.60	6.06
7	Cu2S	1260.000	0.512	81.465	0.015	17.60	6.06
8	Flue dust	1260.000	0.095	12.099	0.003	4.01	-19.20
9	Cu2O	1260.000	0.017	2.415	0.000	0.77	-0.03
10	Fe3O4	1260.000	0.028	6.402	0.001	1.95	-6.64
11	SiO2	1260.000	0.049	2.932	0.001	1.16	-11.19
12	CaO*Al2O3*2SiO2	1260.000	0.001	0.351	0.000	0.13	-1.35
13	Flue gas	1260.000	29.409	981.134	670.287	352.04	121.94
14	SO2(g)	1260.000	2.791	178.779	63.600	50.62	-179.48
15	N2(g)	1260.000	12.393	347.165	282.477	136.23	136.23
16	O2(g)	1260.000	14.225	455.190	324.210	165.20	165.20
17	Flue dust (Conv. 1 return)	1260.000	0.095	12.099	0.003	4.01	-19.20
18	Cu2O	1260.000	0.017	2.415	0.000	0.77	-0.03
19	Fe3O4	1260.000	0.028	6.402	0.001	1.95	-6.64
20	SiO2	1260.000	0.049	2.932	0.001	1.16	-11.19
21	CaO*Al2O3*2SiO2	1260.000	0.001	0.351	0.000	0.13	-1.35
22	Heat loss (Converter I):						10.00

Exit Stream < > BALANCE (2) kmol -3.956 kg 0.000 Nm³ -35.921 kWh 406.46 kWh 0.00

Fig. 13. The OUT2 sheet (Converter I), gives the output from the first part of the converter. The formula $=\text{InCa2} * \text{Analysis!L29}/100$ 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. Figure 14 shows the process layout for the Flash Smelting Furnace process.

"Insert, Graphical Object, ..." selection gives possibility to draw lines, rectangles, etc. on the additional sheets. However, it is recommended to draw flowsheets using "Format, Border, ..." and "Format, Pattern, ..." selection because these properties are more compatible with Excel 95, 97 and 2000. Arrows may be drawn using "Insert, Graphical Object, Arrow" selection.

HSC graphical objects are compatible only with Excel 95. This means that if you want to get the graphical objects to Excel-files then you should save using "File, Save XLS 5 file, ..." dialog.

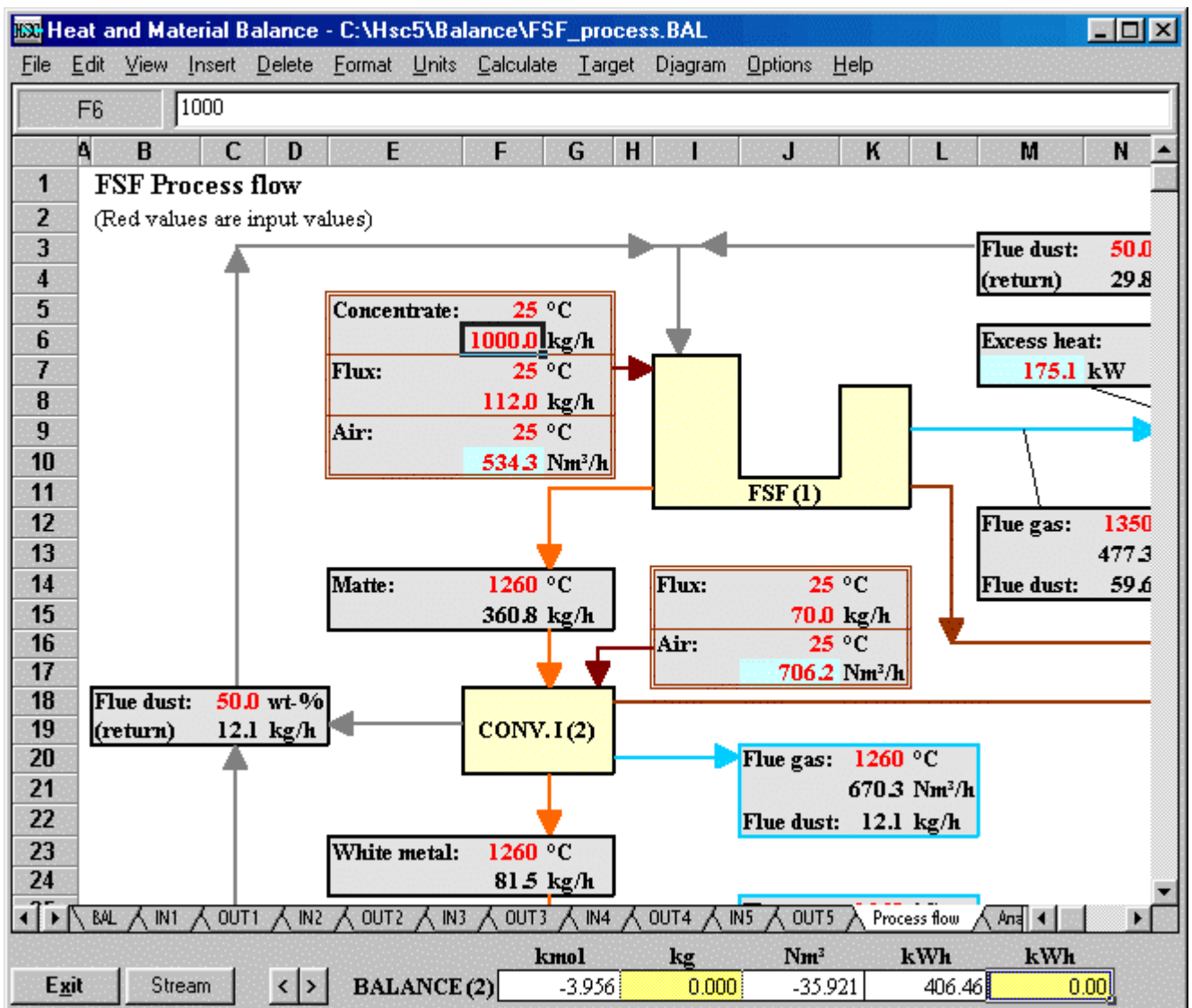


Fig. 14. Process layout and input sheet for the Flash Smelting Furnace process.

Figure 15 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 using the automatically defined names, for example InCa and InO2, and 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.BAL 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 chapter 8. *Target Dialog*.

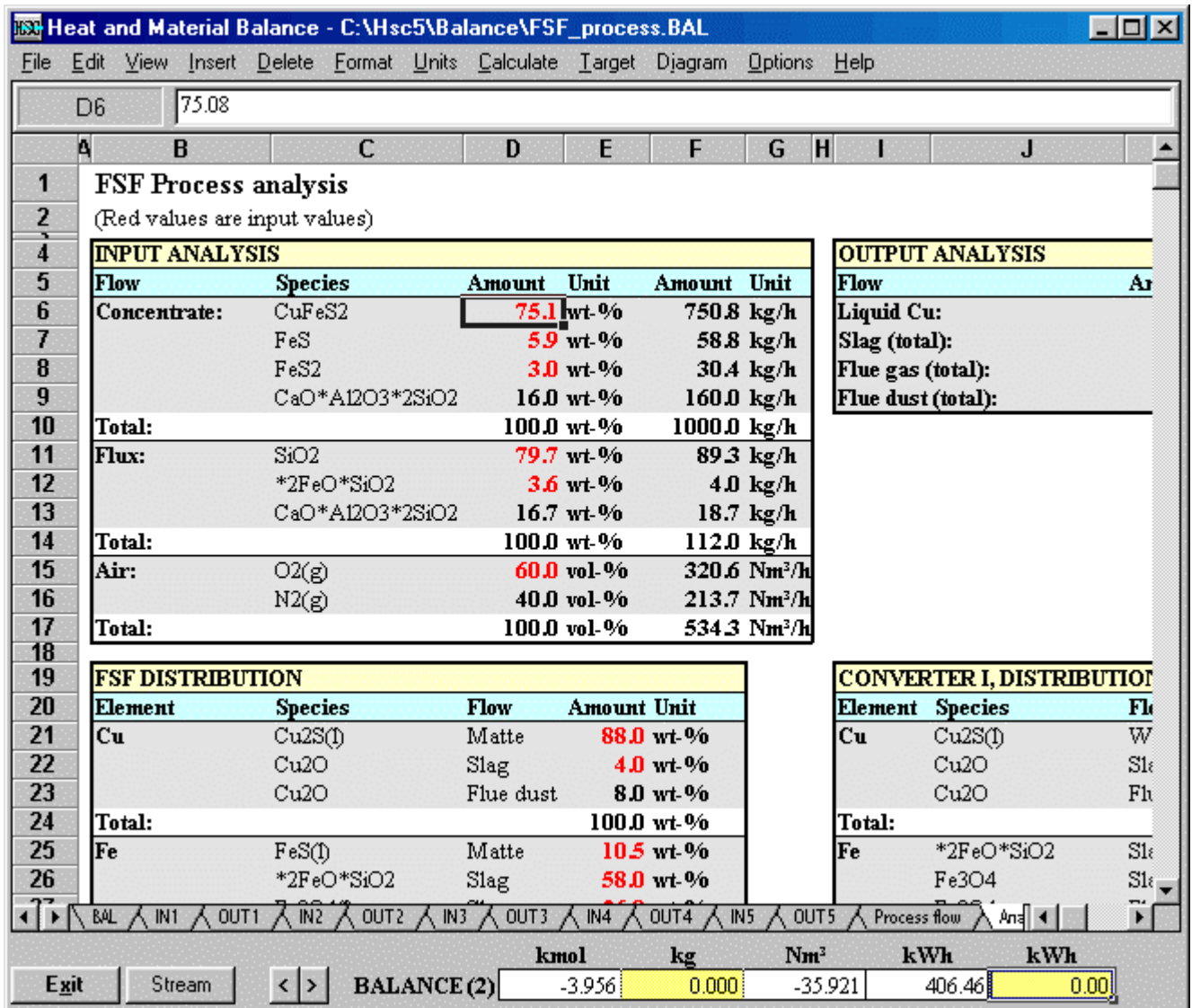


Fig. 15. Detailed analysis of the input and output streams and the elemental distributions into different species. The distributions are given in wt-% (weight percentage).

11.10 General Considerations

In the Heat Balance module it is possible to use the new add-in functions provided by HSC 5.0. The functions should be enabled automatically, this may be seen from the **File** selection in the menu. A checked **HSC5.dll On** indicates that the functions are available and a checked **HSC5.dll Off** indicates that they are disabled. Sometimes it is necessary to browse the location of the add-in file manually. This is done by selecting **File/Add-Ins** from the menu and then browsing to your Windows system directory (for example c:\Windows\System in Windows 98) by pressing the **Browse...** button. Select the file "HSC5.dll". A more detailed description of the functions available may be found in Chapter 27. *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. Notice also 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 **Latent H** 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 heats (= enthalpies of the possible phase transformations) but also specific heats. The enthalpies given in the **Total H** column contain the values of the Latent H column as well as the heats 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 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 Mineralogy Iterations module, see Chapter 22. *Mineralogy iterations*. 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 chapter 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 select some of the ready made files in the directory for editing. HSC 5.0 can read the old HSC 2.0 Heat Balance text-files, but it cannot save them in the old format. The new HSC 5.0 Heat Balance files save all the sheets and formats, not only the text data.

1. Preliminary check for a heat balance (CUSMELT.BAL 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.OHE and CUSMELT.OHE, Fig. 1.

2. Adiabatic temperature of the flame (BUTANE.BAL-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 Calculate/Temperature Balance from the menu, Fig. 3, see example BUTANE.OHE.

3. Dimensioning of an evaporator (H2O.BAL-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 example H2O.OHE.

4. Net and gross heat value of coal, fuel oil and natural gas.

(Coal1-, Coal2-, FuelOil1-, FuelOil2-, NatGas1.bal-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. Notice that the chemical structures of the fuel oil and coal are very complicated, however, heat values based on the elemental analysis will usually give sufficiently accurate results for practical applications.

5. Outokumpu Flash Smelting Furnace process (FSF_process.BAL-file).

This highly simplified process case consist 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 **Process flow** sheet and in the **Analysis** sheet. By pressing **F8** or by selecting **Iterate All** from the **Target Dialog**,

the heat balances are calculated. The values calculated are in the **Process flow** sheet and indicated by a light blue cell background.

6. Iron production process (Iron_process.BAL 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 **Process flow** sheet, with a more detailed analysis available in the **Analysis** sheet. 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.