This document contains Chapter 4 from the book by Chemplant

Data Validation and Reconciliation in Practice

Recon Demo Examples

Mass and Component Balancing

Index

4 Examples of mass and component balances

Let us further give several typical examples of mass and component balances. This chapter will enable the reader to create simple models in the RECON program and check the results.

The structure of all sections is as follows.

1. BALANCE SCHEME. It is a copy of the scheme created in the graphical editor of program RECON.
2. INPUT DATA. It is a somewhat abridged extract from the data of the problem created in program RECON – menu *Flowsheet–Data review - Brief*. It contains all information necessary for the task configuration.
3. RESULTS. It is an abridged extract from the results for the user's inspection, created in program RECON – menu *Calculate –Results*.

Although this manual cannot replace detailed manual to the RECON program, let us still briefly describe the procedure to be maintained in the task creation.

1. Enter the name of the task that is also the name of the task file of the model being created
2. Enter the text of the description (long name) – not obligatory.
3. In the further panel, change the physical units (when necessary). Units selected in individual examples are given in the part INPUT DATA.
4. Enter the names of components (species). In the case of single-component balances, we recommend to enter 'mass'; full name need not be filled in.
5. The graphical editor screen turns up. The scheme drawing proper is recommended to be started by drawing first all nodes, which are conveniently placed on the screen (at later changes in size and placement of the nodes, the shape of the streams drawn can change). Helpful is also a lattice that can be

called up in menu *Settings - Gridlines*. At the nodes, we fill in only Name (it is in the scheme) and Description (one need not to fill it, or we devise some).

6. We then finish by drawing the streams. Their short names are given in the scheme, we invent again the description. Types of streams, values and possible errors (for the measured variables) can be found in part INPUT DATA. The problem definition for mass balance is thus complete.

7. After the configuration of all streams and nodes, one can carry out the computation.

Let us in addition explain certain abbreviations used in the RECON program.

F	type of variable - Fixed variable (known as errorless)
M	type of variable - Measured variable
MC	type of variable - Measured variable, adjustable (can be Corrected)
MN	type of variable - Measured variable, Nonadjustable
N	type of variable - uNmeasured variable
NO	type of variable - uNmeasured variable, Observable
NN	type of variable - uNmeasured variable, uNobservable

For most of the examples given in this chapter, the reader will have at hand also their model solutions, i.e. files with respective models. Names of the files are given in the text.

4.1 Mass balance at steady state without redundancy

In the following four examples, we'll show basic situations that can occur at the data validation. We'll make use of a simple scheme with four nodes and eight streams. One deals with a single-component balance. From the mathematical point of view, one deals with a linear model.

In the first example, in the problem are measured just so many variables how many are necessary for solving the set of balance equations (4 equations for 4 unmeasured variables). The degree of redundancy equals zero and in this case, it is thus impossible to carry out the data validation. The balance scheme is given in the next figure. The full lines represent measured streams, the dash-and dotted ones are unmeasured.

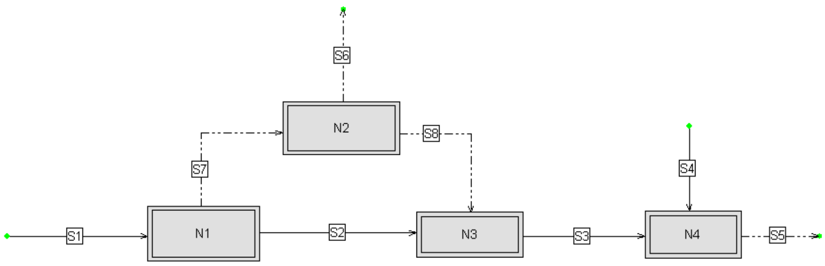


Fig. 4.1-1: Balance scheme (demo Example MC-1)

Input data

ID	TYPE	VALUE	MAX.ERROR
S1	M	100.1000	2.0000 %
S2	M	41.1000	4.0000 %
S3	M	79.0000	2.0000 %
S4	M	30.6000	10.0000 %
S5	N	10.0000	
S6	N	10.0000	
S7	N	10.0000	
S8	N	10.0000	

At the unmeasured variables (type N), their values represent the estimate necessary for starting the computation (so-called initial guess). This value has no influence on the final result. Still, it should be as close as possible to the actual value. The program finds thus easier the solution, and the risk of divergence of the computation process is diminished (this risk can never be quite precluded). As the initial guess, RECON does not accept zero value.

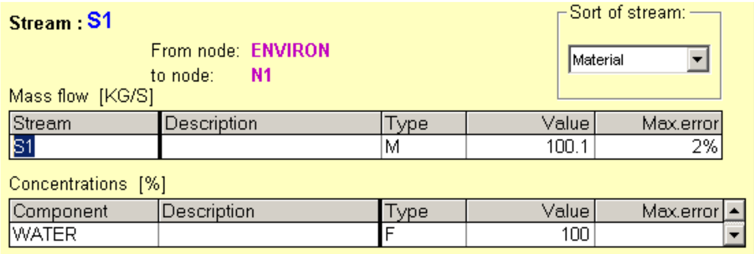


Fig. 4.1-2: Example of stream definition panel

In this panel, we can enter or modify the name of the stream, its description, type (M,N, or F). In case of type M, we must enter the maximum error (absolute or in per cents). In the case of mass (single-component) balance only, the concentration of the one component is always 100 % (obligatorily fixed).

In the next figure, a node property definition is illustrated.

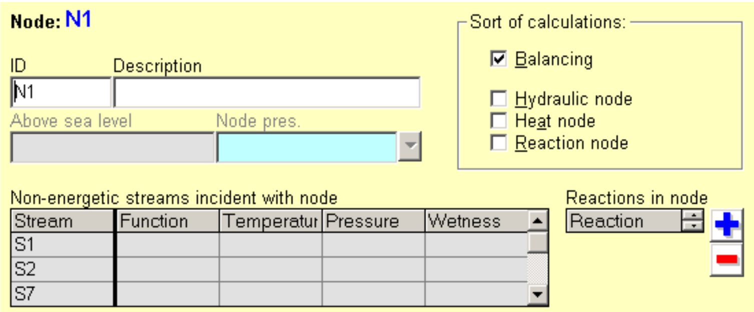


Fig.4.1-3: Illustration of the node definition panel

Here, we again utilize the possibility of entering the name of the node (ID), contingently its description.

RESULTS

```
I T E R A T I O N

Iter            Qeq            Qx              Qy            Qmin

START     2.8722E+01
    1       0.0000E+00     0.0000E+00      2.8748E+01      0.0000E+00
    2       0.0000E+00     0.0000E+00      0.0000E+00      0.0000E+00

  Key:
  Qeq    mean residual of equations
  Qx     mean increment of measured variables in iteration
  Qy     mean increment of unmeasured variables in iteration
  Qmin   least squares function

  G L O B A L   D A T A
  Number of nodes                                   4
  Number of streams                                 8
  Number of components                              1
  Number of measured variables                      4
  Number of adjusted variables                      0
  Degree of redundancy                              0
  Number of unmeasured variables                    4
  Number of observable variables                    4
  Number of unobservable variables                  0
  Number of free variables                          0
  Number of equations                               4
```

```
Number of independent equations          4
Number of user defined equations         0

Mean residual of the equations           0
Qmin                                     0
Qcrit                                    0
Status (Qmin/Qcrit)                      0
```

S T R E A M S [KG/S]

Name	Type	Inp.value	Rec.value	Abs.error
S1	MN	100.100	100.100	2.002
S2	MN	41.100	41.100	1.644
S3	MN	79.000	79.000	1.580
S4	MN	30.600	30.600	3.060
S5	NO	10.000	109.600	3.444
S6	NO	10.000	21.100	2.550
S7	NO	10.000	59.000	2.591
S8	NO	10.000	37.900	2.280

In this first example, let us describe in detail individual information given in the extract.

- Variable *Qeq* is the residual of the equations. The starting value (START) gives the mean quadratic residual of the model equations with the values of measured and estimates (guesses) of unmeasured data.
- Variable *Qx* is mean quadratic increment of measured variables in the iteration. Because one deals with an example without data redundancy, the measured variables need not be adjusted and this value is zero.
- Variable *Qy* is mean quadratic increment of unmeasured variables in the iteration. In the given case (linear model), the values of unmeasured variables are adjusted in just one step (calculated from the measured values). The second iteration is only of checking importance.
- Variable *Qmin* (least squares function) is here zero, as no measured values corrections (adjustments) take place.

The global data need no commentary. Let us perhaps only state the fact that the degree of redundancy is zero, because one does not deal with a redundant system. .

The measured streams are marked by MN, which means that they are Measured and Not corrected (non-adjusted). At unmeasured variables, NO means Non-measured and Observable.

In the results (table Streams), *Inp.value* means measured value or initial estimate for unmeasured variables. *Rec.value* means either adjusted (reconciled) measured value, or computed unmeasured value. In the last column, we have the maximum error of the result.

For example the unmeasured variable S5 was initially estimated (guessed) by the value 10, the computed value was 109.60 and the maximum error was 3.44, all in kg/s. The given value of the error means that the actual (unknown) value lies with probability 95 % in the interval

<109.600 - 3.444; 109.600 + 3.444>.

4.2 Mass balance at steady state with redundancy

The example in the preceding section is modified in the manner that streams No. 5 and 6 are now regarded as measured. This assumption reduces the number of unknowns to 2. As we now have 4 balance equations and 2 unknowns, the degree of redundancy according to Eq. (3.3-1) is 4 – 2 = 2. Some results for this example were already given in Section 3.4 (Example 3.4-1). This information will now be completed.

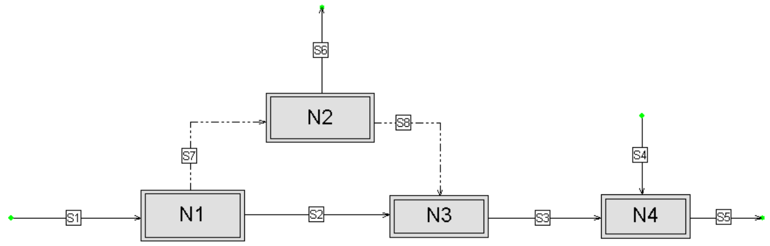


Fig. 4.2-1: Balance scheme (demo Example MC-2)

Dash-and-dotted lines at streams S7 and S8 designate unmeasured streams. The input data are the following:

M A T E R I A L S T R E A M S [KG/S]

ID	TYPE	VALUE	MAX. ERROR
S1	M	100.1000	2.0000 %
S2	M	41.1000	4.0000 %
S3	M	79.0000	2.0000 %
S4	M	30.6000	10.0000 %
S5	M	108.3000	4.0000 %
S6	M	19.8000	4.0000 %
S7	N	10.0000	
S8	N	10.0000	

The results of data reconciliation are:

I T E R A T I O N

Iter	Qeq	Qx	Qy	Qmin
START	1.4944E+01			
1	3.5527E-15	3.0571E-01	2.7931E+01	1.3081E+00
2	3.5527E-15	2.0136E-15	5.1227E-16	1.3081E+00

```
Qeq   mean residual of equations
Qx    mean increment of measured variables in iteration
Qy    mean increment of unmeasured variables in iteration
Qmin  least squares function
```

G L O B A L D A T A

Number of nodes	4
Number of streams	8
Number of components	1
Number of measured variables	6
Number of adjusted variables	5
Degree of redundancy	2
Number of unmeasured variables	2
Number of observable variables	2
Number of unobservable variables	0
Number of free variables	0
Number of equations	4

```
  Number of independent equations                 4
  Number of user defined equations                0

  Mean residual of the equations         3.5527E-15
  Qmin                                   1.3081E+00
  Qcrit                                  5.9739E+00
  Status (Qmin/Qcrit)                      0.218963

S T R E A M S  [KG/S]
```

Name	Type	Inp.value	Rec.value	Abs.error
S1	MC	100.100	99.287	1.300
S2	MN	41.100	41.100	1.644
S3	MC	79.000	79.359	1.239
S4	MC	30.600	30.048	2.533
S5	MC	108.300	109.407	2.632
S6	MC	19.800	19.927	0.755
S7	NO	10.000	58.187	2.096
S8	NO	10.000	38.259	2.058

In the information about the course of computation we see that in contrast to the preceding example, the measured values are now adjusted (column *Qx* in part Iteration). In the second iteration, the increments of variables and residuals are practically zero (given by the number of digits with which the numbers are stored in the computer).

The value of the weighted sum of squares of the adjustments Q_{min} equals 1.308, which is less than the critical value Q_{crit} = 5.9739 (for the chi-square distribution with two degrees of freedom and significance level 95 %). The situation is well characterized by so-called *Status* of the data quality defined by equation (3.11-1), which is the ratio Q_{min}/Q_{crit}. So long as $Q_{min} < Q_{crit}$, the data are in order (no gross error presence detected). In this case, the Status must clearly be smaller than or equal to the value 1.

Concerning this case there are several studies in Chapter 3, which will not be repeated here. Only for brief information:

- enhancing the precision of results as a consequence of reconciliation (Example 3.5-1)
- gross error presence detection (Example 3.6-1)
- gross error identification (Example 3.7-1)
- efficiency of gross errors detection (Example 3.8-1)
- propagation of errors in data processing and measurement system optimization (Example 3.9-2)
- parametric sensitivity (Example 3.10-1).

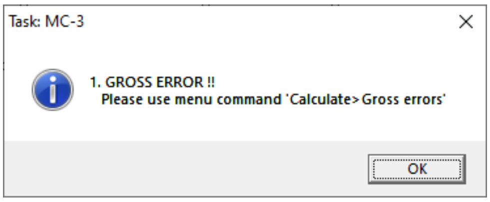
4.3 *Mass balance at steady state with gross error*

This Example is continuation of the preceding Section 4.2. The only change I that to the value of S1 flowrate is added the “Gross Error” +10 kg/s.

M A T E R I A L   S T R E A M S   [KG/S]

ID	TYPE	VALUE	MAX. ERROR
S1	M	110.1000	2.0000 %
S2	M	41.1000	4.0000 %
S3	M	79.0000	2.0000 %
S4	M	30.6000	10.0000 %
S5	M	108.3000	4.0000 %
S6	M	19.8000	4.0000 %
S7	N	10.0000	
S8	N	10.0000	

After the calculation ends, the warning message appears:



The results of data reconciliation are:

```
Task: MC-3 (one-component balance with gross error)

 I T E R A T I O N S

 Iter              Qeq              Qx              Qy              Qmin
 -----------------------------------------------------------------
 START      1.9968E+01
    1       4.3512E-15     1.7168E+00      3.6467E+01      6.4542E+01
    2       2.5121E-15     2.3628E-15      2.5588E-15      6.4542E+01

 Legend:

 Qeq   mean residual of equations
 Qx    mean increment of measured variables in iteration
 Qy    mean increment of non-measured variables in iteration
 Qmin  least-square function


 G L O B A L   D A T A

 Number of nodes                                          4
 Number of streams                                        8
 Number of components                                     1

 Number of measured variables                             6
 Number of adjusted variables                             5
 Number of non-measured variables                         2
 Number of observed variables                             2
 Number of non-observed variables                         0
 Number of free variables                                 0
 Number of equations                                      4
 Number of independent equations                          4
 Number of user-defined equations                         0

 Degree of redundancy                                     2
```

```
Mean residue of equations                              0
Qmin                                          6.4542E+01
Qcrit                                         5.9900E+00
Status (Qmin/Qcrit)                           1.0775E+01


WARNINGS

1. GROSS ERROR !!
   Please use menu command 'Calculate>Gross errors'


M A S S   F L O W R A T E S

Name             Type      Inp.value      Rec.value      Abs.error
------------------------------------------------------------------
S1               MC          110.100        102.981          1.350  KG/S
S2               MN           41.100         41.100          1.644  KG/S
S3               MC           79.000         82.260          1.271  KG/S
S4               MC           30.600         29.082          2.535  KG/S
S5               MC          108.300        111.342          2.639  KG/S
S6               MC           19.800         20.721          0.759  KG/S
S7               NO            1.000         61.881          2.127  KG/S
S8               NO            1.000         41.160          2.078  KG/S
```

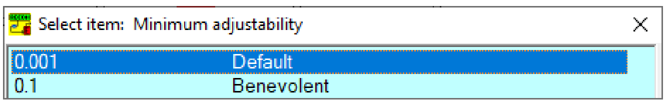
Also the next error file appears:

```
ERRORS / WARNINGS
=================

S U S P E C T   M A S S   I M B A L A N C E S

MACRONODE:
  [ N1, N2, N3 ]

INPUTS:
Stream     From node  To node                Value            Error
-------------------------------------------------------------------
S1         ENVIRON    N1                     110.1            2.202 KG/S
                                  ----------------
           Sum of inputs:                    110.1

OUTPUTS:
Stream     From node  To node                Value            Error
-------------------------------------------------------------------
S6         N2         ENVIRON                 19.8            0.792 KG/S
S3         N3         N4                        79             1.58 KG/S
                                  ----------------
           Sum of outputs:                    98.8

           Imbalance:                         11.3 (10.8%)
           Test (should be < 1.96):          7.844
```

This is the balance of the macronode N1, N2 and N3.

The value of the weighted sum of squares of the adjustments Q_{min} equals 64.542, which is more than the critical value Q_{crit} = 5.9739 (for the chi-square distribution with two degrees of freedom and significance level 95 %). The situation is well characterized by so-called *Status* of the data quality defined by equation (3.11-1), which is the ratio Q_{min}/Q_{crit}. Which is 10.775. As the Status is greater than 1, some gross error is detected.

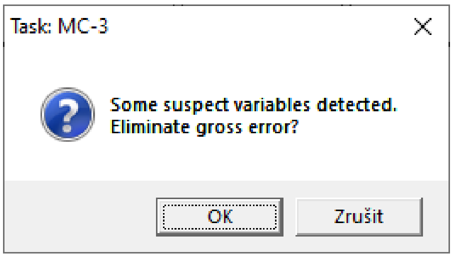
Let’s now visit the menu *Calculate/Gross errors.* The following selection box appears:



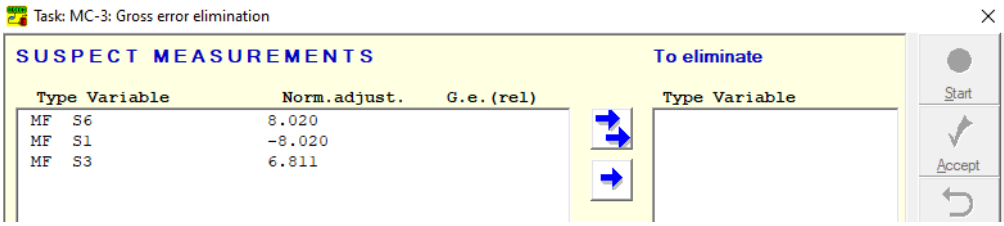
In this small example you can select any choice. In large tasks the selection *Benevolent* narrows the list of suspect variables. The following text appears:

```
REPORT ON GROSS ERRORS
 =====================

 S U S P E C T   M E A S U R E M E N T S

  Type Variable Importance  G.e.(abs)  Meter     Meas.     Calc.    Diff.  Unit  Description
  -------------------------------------------------------------------------------------------
   MF   S6           8.020       11.3            19.800    20.721    0.921  KG/S
   MF   S1          -8.020       11.3           110.100   102.981   -7.119  KG/S
   MF   S3           6.811       10.7            79.000    82.260    3.260  KG/S

 Status >= 10.77
 Adjustability >= 0.001

 Legend:
  Importance   = normalized adjustment
                 (big value => suspect as gross error)
  G.e.(abs)    = estimated gross error (absolute value)
  Meter        = Import tag
  Meas.        = Measured data
  Calc.        = Reconciled data
  Diff.        = Reconciled data minus Measured data

  MF   Mass flow
```

The most informative is the column *Importance*. Suspect variables (S6, S1 and S3) are aligned according to their normalized adjustments. After closing this information box you are asked:

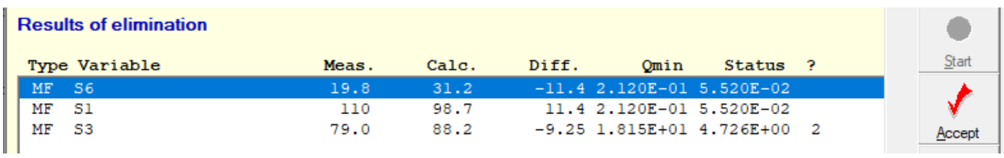


By selecting OK you enter the Gross Error elimination process:



Type	Variable	Norm.adjust.	G.e.(rel)
MF	S6	8.020	
MF	S1	-8.020	
MF	S3	6.811	

Here you can put the suspect measured variables one by one among unmeasured variables and repeat the data reconciliation. By pressing the blue double arrow you can try it on all suspect variables. Then press the *Start* button. Recon then puts S6, S1 and S3 one by one among unmeasured ones and calculates the new data reconciliations.



Type	Variable	Meas.	Calc.	Diff.	Qmin	Status	?
MF	S6	19.8	31.2	-11.4	2.120E-01	5.520E-02	
MF	S1	110	98.7	11.4	2.120E-01	5.520E-02	
MF	S3	79.0	88.2	-9.25	1.815E+01	4.726E+00	2

The most informative is the column *Status*. It informs us that only the elimination of S1 and S6 has got the Status below 1. This means that flowrates S1 and S6 remain the only suspects as the cause

4.4 Mass balance at steady state with unobservable variables

The aim of this example is to show the consequences of insufficient instrumentation of the measurement system.

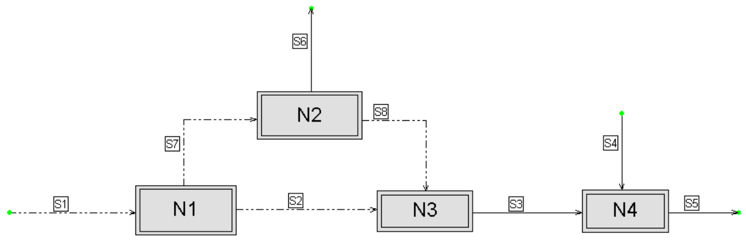


Fig. 4.4-1: Balance scheme (demo Example MC-4)

We have here 4 unmeasured streams (dash-and-dotted), so one could believe that they could be computed from the 4 balance equations. The input data are:

M A T E R I Á L S T R E A M S [KG/S]

ID	TYPE	VALUE	MAX.ERROR
S1	N	100.1000	
S2	N	41.1000	
S3	M	79.0000	2.0000 %
S4	M	30.6000	10.0000 %
S5	M	108.3000	4.0000 %
S6	M	19.8000	4.0000 %
S7	N	10.0000	
S8	N	10.0000	

The abridged results read:

```
Number of measured variables                    4
Number of adjusted variables                    3
Degree of redundancy                            1
Number of unmeasured variables                  4
Number of observable variables                  1
Number of unobservable variables                3
Number of free variables                        1
Number of equations                             4
Number of independent equations                 4

W A R N I N G
1. Some unobservable variables detected.
   Please, use menu item 'Calculate > Classification'
```

S T R E A M S [KG/S]

Name	Type	Inp.value	Rec.value	Abs.error
S1	NO	100.100	98.694	1.709
S2	NN	UNOBSERVABLE		
S3	MC	79.000	78.894	1.514
S4	MC	30.600	30.203	2.550
S5	MC	108.300	109.097	2.696
S6	MN	19.800	19.800	0.792
S7	NN	UNOBSERVABLE		
S8	NN	UNOBSERVABLE		

Here, the situation differs from the case examined in Section 4.1. We have now met with the situation where in one part of the scheme, the measurement is quite sufficient and redundancy occurs (around node N4), while in other places, there is lack of measurement (around nodes N1, N2, N3). This can be met in practice quite often, because certain regions of production units are, due to their importance, endowed with meters considerably more than regions of smaller importance. The consequence is then the notice (warning) in the extract from the program, viz. that unobservable variables are present.

Let us first observe that in this case, there no longer holds the relation (3.3-1) that under certain circumstances enables us computing the degree of redundancy. This relation gives degree of redundancy 0 (no redundancy), while in reality all streams connected with node N4 are measured, and also reconciled.

In the basic information on the results, there is the item *Number of free variables* ; this is the necessary number of unmeasured variables to be measured or otherwise fixed, so as to make all variables observable. In the given case, the number of free variables is 1, thus just one unmeasured variable must be given (preferably measured) in addition to make the system fully observable. The selection of this variable is, however, not arbitrary. The problem is solved by the RECON program in menu *Calculations – Classification*. The result reads as follows.

```
U N O B S E R V A B L E   V A R I A B L E S

Type Variable

  MF  S2
  MF  S7
  MF  S8

  Unobservable variables: 3
  1 must be measured or fixed
```

Among the given streams S2, S7, S8, we can choose. Let us note that it makes no sense to measure in addition the further unmeasured stream S1. If we did so, the observability problem would not be solved, only the degree of redundancy is increased (as the reader can verify).

4.5 Mass balance at steady state – an unsolvable system

Besides the variables of types M (measured) and N (not measured), the program RECON knows also so-called *fixed* variables thus constants that do not change in the course of data processing. They also can be conceived as measured variables, with null error. Because the program cannot freely manipulate with their values, in certain situations the data reconciliation process cannot be brought to end (to attain zero residuals). Such a case takes place with the following scheme.

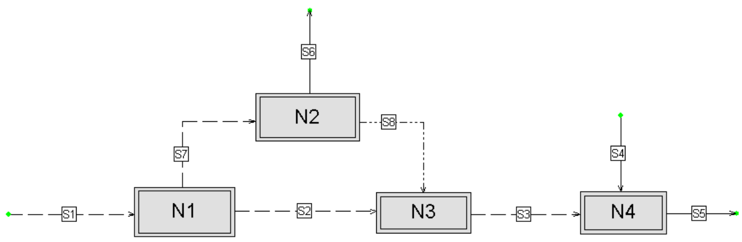


Fig. 4.5-1: Balance scheme (demo Example MC-5)

The dashed lines represent here fixed streams. It is obvious at first sight that in the node N1 balance, only fixed streams occur. If the values of their flowrates are chosen arbitrarily, the balance around this node will most likely not be satisfied. The input data are following.

M A T E R I A L   S T R E A M S   [KG/S]

ID	TYPE	VALUE	MAX.ERROR
S1	F	100.1000	
S2	F	41.1000	
S3	F	79.0000	
S4	M	30.6000	10.0000 %
S5	M	108.3000	4.0000 %
S6	M	19.8000	4.0000 %
S7	F	58.0000	
S8	N	10.0000	

During the computation with these data, the following results turn up.

I T E R A T I O N

Iter	Qeq	Qx	Qy	Qmin
START	9.9258E+00			
1	2.5000E-01	3.3809E-01	2.7900E+01	7.8199E-01
2	2.5000E-01	4.2509E-15	0.0000E+00	7.8199E-01
3	2.5000E-01	4.2509E-15	0.0000E+00	7.8199E-01
4	2.5000E-01	4.2509E-15	0.0000E+00	7.8199E-01
5	2.5000E-01	4.2509E-15	0.0000E+00	7.8199E-01

Task does not converge !!!

It is seen that one has not been able to attain zero residuals of the equations. If employing the service of menu *Calculate – Solvability*, we obtain the following message.

```
MESSAGE ON SOLVABILITY
The following fixed variables are not consistent:

 Type of variable

  MF  S1
  MF  S2
  MF  S7

 Legend:
  MF  Mass flow

 Note
From these variables 1 must be re-classified to 'M' (measured) or 'N' (unmeasured)
Please correct your task.
```

4.6 Multicomponent balance of the LPG separation

The mixture of hydrocarbons LPG (Liquefied Petroleum Gas) is separated in the system of three distillation columns

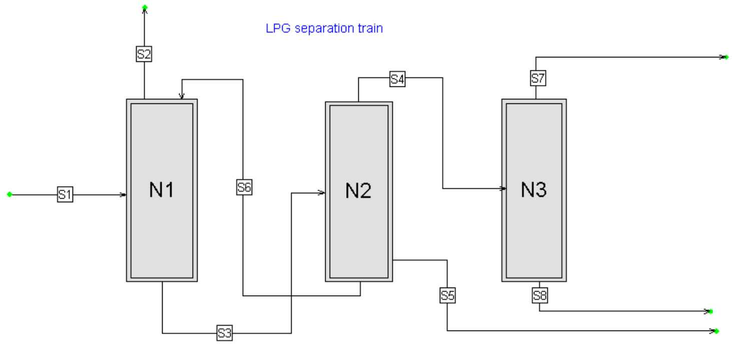


Fig. 4.6-1: Balance scheme (demo example MC-6)

We have here altogether 5 components, 3 balancing nodes (distillation columns) and 8 streams.

Components:	C1	ethane
	C2	propane
	C3	i-butane
	C4	n-butane
	C5	pentane+ (pentane and higher hydrocarbons)

The hydrocarbon mixture S1 is led into node N1, so-called absorber – desorber. In its upper part, heavier hydrocarbons are stripped by the pentane fraction S6 , giving rise to so-called lean (residual) gas consisting mainly of ethane. In column N2, hydrocarbons C4 and lighter (stream S4) are separated from pentane and heavier hydrocarbons (streams S5 and S6). In column N3, propane (stream S7) is separated from the butanes (stream S8).

All flowrates and their composition are measured with the exception of the stream S3 composition. The maximum errors at the measurement of concentrations are expressed as so-called *relative per cents* , i.e. per cents from the concentration measured itself also in per cents. The input data read as follows.

```
M A T E R I A L   S T R E A M S  [kg/h],  [%]

 ID          COMPONENT   TYPE          VALUE     MAX.ERROR

 S1            Flowrate    M       8620.0000      4.0000 %
               C1         M         10.500000    5.000000 %
               C2         M         32.000000    3.000000 %
               C3         M         43.600000    3.000000 %
               C4         M          3.000000   15.000000 %
               C5         M          9.500000    5.000000 %

 S2            Flowrate   M       1040.0000      6.0000 %
               C1         M         85.700000    2.000000 %
               C2         M          2.100000   15.000000 %
               C3         M          2.300000   15.000000 %
               C4         M          1.300000   15.000000 %
               C5         M          9.900000    5.000000 %

 S3            Flowrate   M      17800.0000      4.0000 %
               C1         N          0.100000
```

	C2	N	15.000000	
	C3	N	20.000000	
	C4	N	5.000000	
	C5	N	60.000000	
S4	Flowrate	M	6860.0000	4.0000 %
	C1	M	0.200000	40.000000 %
	C2	M	41.200000	3.000000 %
	C3	M	54.200000	3.000000 %
	C4	M	2.700000	5.000000 %
	C5	M	0.600000	40.000000 %
S5	Flowrate	M	810.0000	2.0000 %
	C1	F	0.00000E+0	
	C2	M	0.400000	40.000000 %
	C3	M	1.800000	15.000000 %
	C4	M	8.200000	5.000000 %
	C5	M	90.200000	1.000000 %
S6	Flowrate	M	10400.0000	4.0000 %
	C1	F	0.00000E+0	
	C2	F	0.00000E+0	
	C3	M	0.200000	40.000000 %
	C4	M	3.300000	15.000000 %
	C5	M	95.900000	0.500000 %
S7	Flowrate	M	2850.0000	2.0000 %
	C1	M	0.600000	40.000000 %
	C2	M	96.200000	0.500000 %
	C3	M	3.700000	15.000000 %
	C4	F	0.00000E+0	
	C5	F	0.00000E+0	
S8	Flowrate	M	4060.0000	2.0000 %
	C1	M	0.100000	40.000000 %
	C2	M	2.500000	15.000000 %
	C3	M	91.400000	1.000000 %
	C4	M	4.500000	5.000000 %
	C5	M	0.700000	40.000000 %

At the configuration of this problem, we must first enter the components C1 to C5. The full name is not filled in.

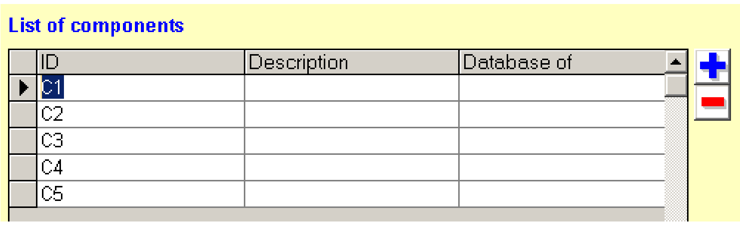


Fig. 4.6-2: Panel for components definition

At the creation of streams, besides the flowrates one also fills in the component concentrations.

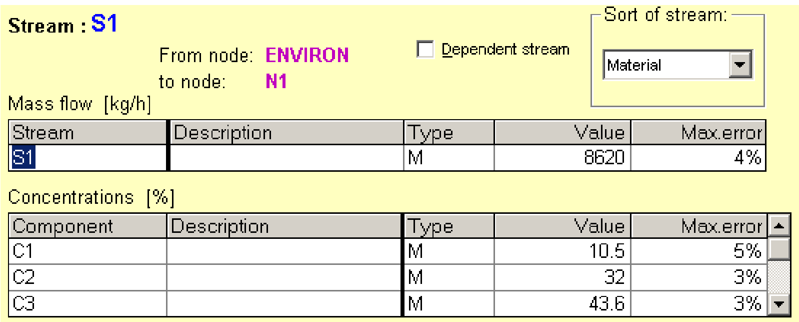


Fig. 4.6-3: Panel for filling-in the streams parameters

We further give the extract of the results. At the stream properties, for the sake of space we restrict ourselves to one stream.

```
Problem: MC-6 (Component balance of system of 3 dist. columns)

 I T E R A T I O N

  Iter          Qeq           Qx              Qy            Qmin


  START    6.6866E-03
    1      7.9806E-05    5.5151E-04      4.6870E-03      2.1447E+01
    2      1.5241E-09    1.9499E-06      5.5365E-05      2.1364E+01

  Key:
  Qeq   mean residual of equations
  Qx    mean increment of measured variables in iteration
  Qy    mean increment of unmeasured variables in iteration
  Qmin  least squares function

  G L O B A L   D A T A

  Number of nodes                                  3
  Number of streams                                8
  Number of components                             5
  Number of measured variables                    38
  Number of adjusted variables                    38
  Degree of redundancy                            18
  Number of unmeasured variables                   5
  Number of observable variables                   5
  Number of unobservable variables                 0
  Number of free variables                         0
  Number of equations                             23
  Number of independent equations                 23
  Number of user defined equations                 0
  Mean residual of the equations                 1.5241E-09
  Qmin                                           2.1364E+01
  Qcrit                                          2.8919E+01
  Status (Qmin/Qcrit)                            0.738748

  S T R E A M S    [kg/h],  [%]

  Name of stream:  S1
  No. Name       Type        Inp.value       Rec.value       Abs.error

  Flowrate   MC          8620.000       8756.334        102.642
   1  C1         MC          10.500          10.429           0.368
   2  C2         MC          32.000          32.677           0.413
   3  C3         MC          43.600          44.048           0.459
   4  C4         MC           3.000           3.017           0.084
   5  C5         MC           9.500           9.829           0.196
```

4.7 Component balance of the chlorination of methane

The following section describes the balance of a single node – reactor – where several chemical reactions take place.

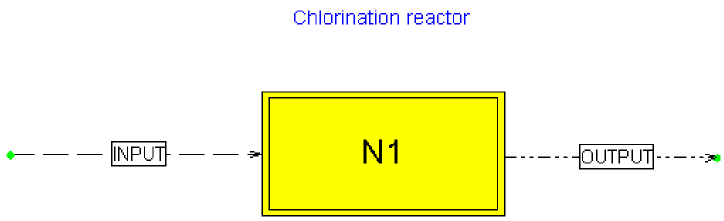


Fig. 4.7-1: Balance scheme (demo example MC-7)

Let us consider the chlorination of methane. From the balancing point of view, altogether 7 components occur in the system (the balancing viewpoint means that one ignores intermediate reaction products, radicals etc., which may participate in the reactions but do not belong to the initial reaction species, nor to the products):

Component No.	Formula
1	Cl_2
2	CH_4
3	CH_3Cl
4	CH_2Cl_2
5	$CHCl_3$
6	CCl_4
7	HCl

The chlorination reactor has one inlet and one outlet stream. For the seven components, four independent stoichiometric equations can be written.

$$\begin{aligned} Cl_2 + CH_4 - CH_3Cl - HCl &= 0 \\ Cl_2 + CH_3Cl - CH_2Cl_2 - HCl &= 0 \\ Cl_2 + CH_2Cl_2 - CHCl_3 - HCl &= 0 \\ Cl_2 + CHCl_3 - CCl_4 - HCl &= 0 \end{aligned} \quad (4.6\text{-}1)$$

The set of equations (4.6-1) constitutes so-called *maximal set of stoichiometric equations* for the given system of species. Any further reaction must be linearly dependent on the above equations (it can be formed as a linear combination of the latter) . For example the stoichiometric equation

$$2Cl_2 + CH_4 - CH_2Cl_2 - 2\,HCl = 0 \quad (4.6\text{-}2)$$

is sum of the first two equations in (4.6-1). We'll return later to the problem that would arise, if we added this equation to the maximal set and wanted then use it in the balancing.

Let us now go back to the original problem formulation in the RECON program. We first give the components occurring in the problem.

List of components

ID	Description	Database of
Cl2		
CH4		
CH3Cl		
CH2C2		
CHCl3		
CCl4		
HCL		

Fig. 4.7-2: Panel for defining the components

Further, we have to enter the values of flowrates and concentrations.

M A T E R I A L S T R E A M S [mol/s], [%]

ID	COMPONENT	TYPE	VALUE	MAX.ERROR
INPUT	Flowrate	M	100.0000	3.0000 %
	Cl2	M	62.100000	10.000000 %
	CH4	M	26.900000	10.000000 %
	CH3Cl	M	10.800000	10.000000 %
	CH2C2	M	0.780000	10.000000 %
	CHCl3	M	0.380000	10.000000 %
	CCl4	F	0.00000E+0	
	Cl2	F	0.00000E+0	
OUTPUT	Flowrate	N	100.0000	
	Cl2	F	0.00000E+0	
	CH4	M	1.570000	10.000000 %
	CH3Cl	M	6.830000	10.000000 %
	CH2C2	M	24.800000	10.000000 %
	CHCl3	M	4.820000	10.000000 %
	CCl4	M	0.390000	10.000000 %
	Cl2	M	59.300000	10.000000 %

Our reactor is a laboratory one, where only samples of inlet and outlet streams are taken and analyzed. The flowrate is measured at the inlet only. One sets up the material balance in units of species (matter) variable. After entering the properties of streams, one has to enter information on the chemical reactions. This is done in two steps. First, one creates so-called *reaction bank*.

List of reactions

Heat of reaction: Positive for exothermic reactions, [KJ/mol]
Stoich.coefficients: Positive for reactants, negative for products

ID	Description	Heat	Cl2	CH4	CH3Cl	CH2C2	CHCl3	CCl4	HCL
R1		0	1	1	-1	0	0	0	-1
R2		0	1	0	1	-1	0	0	-1
R3		0	1	0	0	1	-1	0	-1
R4		0	1	0	0	0	1	-1	-1

Fig. 4.7-3: Panel for creating the reaction bank

In the second step, with the reaction nodes one associates the reactions defined in the bank.

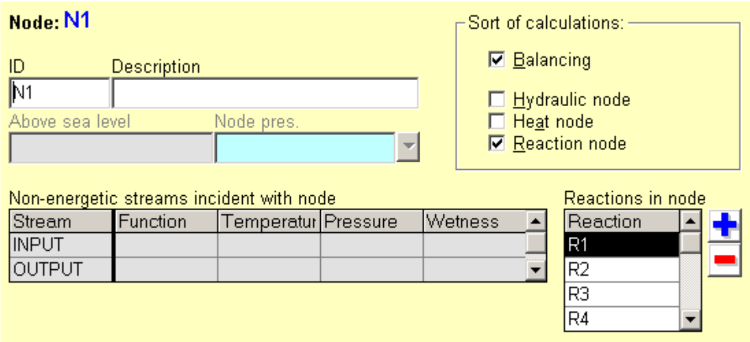


Fig. 4.7-4: Associating reactions with reaction node

At the panel of node in Fig. 4.6-4, we first mark the window *Reaction node* on the right above. One then can choose a reaction from the list in the reaction bank.

The data input is thus finished. The results of the data reconciliation are following:

G L O B A L   D A T A

Number of nodes	1
Number of streams	2
Number of components	7
Number of reactions	4
Number of reaction nodes	1
Number of measured variables	12
Number of adjusted variables	11
Degree of redundancy	4
Number of unmeasured variables	5
Number of observable variables	5
Number of unobservable variables	0
Number of free variables	0
Number of equations	9
Number of independent equations	9
Number of user defined equations	0
Mean residual of the equations	4.9403E-07
Qmin	9.4573E-01
Qcrit	9.5145E+00
Status (Qmin/Qcrit)	0.099400

S T R E A M S   [mol/s], [%]

Name of stream: INPUT

No.	Name	Type	Inp.value	Rec.value	Abs.error
	Flowrate	MN	100.000	100.000	3.000
1	Cl2	MC	62.100	60.716	0.463
2	CH4	MC	26.900	27.328	0.742
3	CH3Cl	MC	10.800	10.797	1.031
4	CH2C2	MC	0.780	0.780	0.078
5	CHCl3	MC	0.380	0.380	0.038
6	CCl4	F	0.00E+0	0.00E+0	
7	Cl2	F	0.00E+0	0.00E+0	

Name of stream: OUTPUT

No.	Name	Type	Inp.value	Rec.value	Abs.error
	Flowrate	NO	100.000	99.993	3.000
1	Cl2	F	0.00E+0	0.00E+0	
2	CH4	MC	1.570	1.570	0.157
3	CH3Cl	MC	6.830	6.862	0.670
4	CH2C2	MC	24.800	25.598	0.818
5	CHCl3	MC	4.820	4.864	0.466
6	CCl4	MC	0.390	0.390	0.039
7	Cl2	MC	59.300	60.716	0.463

```
R R E A C T I O N   E X T E N T S

Node       Reaction          Extent

N1          R1              25.756
            R2              29.691
            R3               4.875
            R4               0.390
```

Let us go back once more to the problems concerning the set of stoichiometric reactions used in the balancing. To the set of equations (4.6-1), let us add the dependent equation (4.6-2). The reaction bank is then of the form

List of reactions

Heat of reaction: Positive for exothermic reactions, [KJ/mol]
Stoich.coefficients: Positive for reactants, negative for products

ID	Description	Heat	Cl2	CH4	CH3Cl	CH2C2	CHCl3	CCl4	HCL
R1		0	1	1	-1	0	0	0	-1
R2		0	1	0	1	-1	0	0	-1
R3		0	1	0	0	1	-1	0	-1
R4		0	1	0	0	0	1	-1	-1
R5		0	2	1	0	-1	0	0	-2

If we associate all these 5 reactions with reactor N1, the computation will run with the result that certain reaction extents remain unobservable.

```
R E A C T I O N   E X T E N T S

Node       Reaction         Extent

N1         R1             UNOBSERVABLE
             R2             UNOBSERVABLE
             R3              4.875
             R4              0.390
             R5             UNOBSERVABLE
```

All other results remain however the same as before adding the dependent reaction (4.6 2). This means only that the extents of the dependent reactions cannot be identified by the measured data (although all the reactions can run in the given species system). On the other hand, if some of the independent reactions of the set (4.6-1) were considered absent, the results would change and probably, the presence of a gross error would be detected.

4.8 *Ammonia synthesis reactor – master and dependent streams*

The following section describes the multi-component balance of a reactor for synthesis of ammonia.

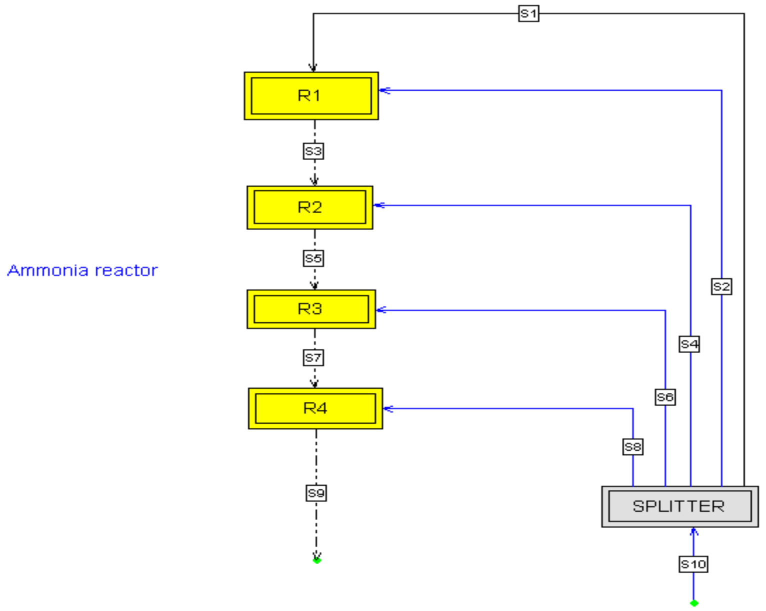


Fig. 4.8-1: Balance flow-sheet (demo example MC-8)

The synthesis gas (stream S10) consists of four components:

Component No	Formula
1	H_2
2	N_2
3	NH_3
4	CH_4Ar

The pseudocomponent CH_4Ar represents inert species in the synthesis gas, mostly methane and rare gases (stemming from the technology of its preparation).

The ammonia reactor has four beds (sections). The reactants from sections are quenched by introducing parts of the cold raw synthesis gas (streams S2, S4, S6 and S6). There is only one chemical reaction in the system:

$$3H_2 + N_2 - 2NH_3 \quad = 0 \qquad (4.7\text{-}1)$$

Let us now go back to the original problem formulation in the RECON program. We first define the components occurring in the problem.

This reaction must be put into the reaction bank and associated with reactors R1, R2, R3 and R4 in the way described in the preceding example.

There are 6 streams incident with the SPLITTER node (S1, S2, S4, S6, S8 and S10). These streams have the same composition. We can select for example the S1 stream as the *master* stream, the 5 remaining streams will be so-called *dependent* streams – see Subsection 2.3.2 (the choice of the master stream is arbitrary and does not influence the results).

Concentrations are entered only for the master stream, the dependent streams are only marked as dependent on their panel of parameters.

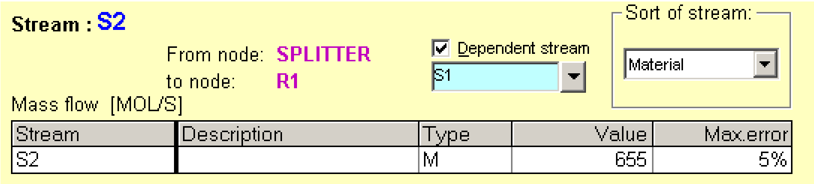


Fig. 4.8-2: Panel for defining a dependent stream

Further, we have to enter the values of flowrates and concentrations.

```
M A T E R I A L   S T R E A M S   [MOL/S],  [%]

 ID           COMPONENT  TYPE        VALUE     MAX.ERROR

 S1           Flowrate    M       655.0000      5.0000 %
              H2          M        63.800000    2.000000 %
              N2          M        21.100000    2.000000 %
              NH3         M         3.000000    2.000000 %
              CH4AR       M        12.000000    2.000000 %

 S10          Flowrate    M      2300.0000      5.0000 %
Composition identical with stream 'S1'

 S2           Flowrate    M       655.0000      5.0000 %
Composition identical with stream 'S1'

 S3           Flowrate    N      1200.0000
              H2          M        57.200000    2.000000 %
              N2          M        19.000000    2.000000 %
              NH3         M        10.900000    2.000000 %
              CH4AR       M        12.900000    2.000000 %

S4           Flowrate    M        330.0000      5.0000 %
Composition identical with stream 'S1'

 S5           Flowrate    N      1400.0000
              H2          M        53.400000    2.000000 %
              N2          M        17.700000    2.000000 %
              NH3         M        15.400000    2.000000 %
              CH4AR       M        13.500000    2.000000 %

S6           Flowrate    M        360.0000      5.0000 %
Composition identical with stream 'S1'

 S7           Flowrate    N      1800.0000
              H2          M        51.700000    2.000000 %
              N2          M        17.100000    2.000000 %
              NH3         M        17.500000    2.000000 %
              CH4AR       M        13.700000    2.000000 %

S8           Flowrate    M        300.0000      5.0000 %
Composition identical with stream 'S1'

 S9           Flowrate    N      2000.0000
              H2          M        51.700000    2.000000 %
              N2          M        16.800000    2.000000 %
              NH3         M        18.700000    2.000000 %
              CH4AR       M        13.800000    2.000000 %
```

The data input is thus finished. The results of the data reconciliation are following (abbreviated):

```
G L O B A L   D A T A

  Number of nodes                              5
  Number of streams                           10
  Number of components                         4
  Number of reactions :                        1
  Number of react. nodes :                     4
  Number of measured variables                26
  Number of adjusted variables                26
  Number of non-measured variables             8
  Number of observable variables               8
  Number of unobservable variables             0
  Number of free variables                     0
  Number of equations                         22
  Number of independent equations             22
  Number of user equations                     0
  Degree of redundancy                        14

  Mean residue of equations           5.8649E-12
  Qmin                                3.5910E+00
  Qcrit                               2.3697E+01
  Status (Qmin/Qcrit)                   0.151541

  S T R E A M S    [MOL/S],  [%]

  Stream name:  S1
  From node 'SPLITTER' to node 'R1'
  No. Name        Type       Inp.value      Rec.value      Abs.error

      Flowrate   MC          655.000        654.835         31.647
   1  H2         MC           63.800         63.854          0.175
   2  N2         MC           21.100         21.149          0.142
   3  NH3        MC            3.000          3.000          0.060
   4  CH4AR      MC           12.000         11.996          0.106

Stream name:  S2
  From node 'SPLITTER' to node 'R1'
  Composition identical with stream 'S1'

  No. Name        Type       Inp.value      Rec.value      Abs.error
      Flowrate   MC          655.000        654.835         31.647

  Stream name:  S3
  From node 'R1' to node 'R2'

  No. Name        Type       Inp.value      Rec.value      Abs.error
      Flowrate   NO         1200.000       1216.440         40.141
   1  H2         MC           57.200         57.252          0.254
   2  N2         MC           19.000         18.938          0.161
   3  NH3        MC           10.900         10.895          0.212
   4  CH4AR      MC           12.900         12.916          0.116
Etc.

E X T E N T S   O F   R E A C T I O N S

  NODE      REACTION      EXTENT
  R1        R1            46.615
  R2        R1            41.528
  R3        R1            35.245
  R4        R1            27.795
```

4.9 Multicomponent balance of a flotation circuit

This example from mineral industry describes the multi-component balance of a flotation circuit (adapted from H.W.Smith and N.M.Ichiyen: *Computer Adjustment of Metallurgical Balances. CIM Bulletin for September, 1973, pp. 97-100*).

Copper and zinc are separated from suspensions by flotation in the following process:

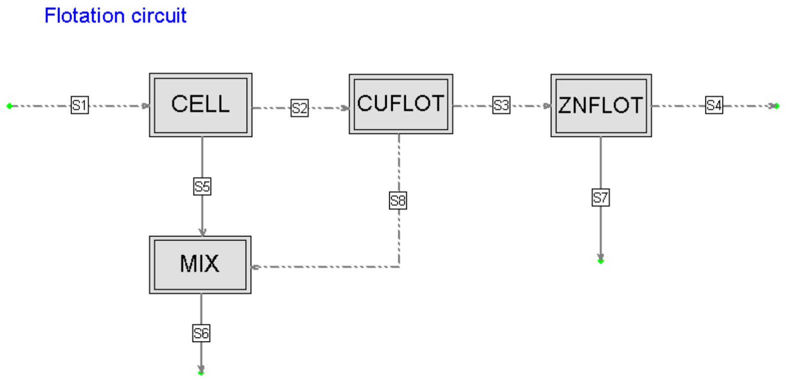


Fig. 4.9-1: Balance flow-sheet (demo example MC-9)

The composition of all streams is simplified to 3 components:

Component No	Formula
1	Cu
2	Zn
3	REST

The pseudocomponent REST represents the remaining elements in the system, including water. The concentration of the REST is always unmeasured and completes the composition to 100 %.

Further are values of flowrates and concentrations.

M A T E R I A L   S T R E A M S   [T/H], [%]

ID	COMPONENT	TYPE	VALUE	MAX.ERROR
S1	Flowrate	N	9.0000	
	CU	M	5.210000	2.00000E-2
	ZN	M	5.410000	2.00000E-2
	REST	N	95.000000	
S2	Flowrate	N	8.0000	
	CU	M	0.450000	5.00000E-2
	ZN	M	4.920000	0.200000
	REST	N	95.000000	
S3	Flowrate	N	7.0000	
	CU	M	0.130000	2.00000E-2
	ZN	M	5.120000	0.200000
	REST	N	95.000000	
S4	Flowrate	N	6.0000	
	CU	M	9.00000E-2	1.00000E-2
	ZN	M	0.410000	2.00000E-2

```
            REST        N          99.000000

S5          Flowrate    M           2.2100    10.0000 %
            CU          M          19.860000    2.000000
            ZN          M           7.090000    1.000000
            REST        N          75.000000

S6          Flowrate    M           2.5000    10.0000 %
            CU          M          21.440000    2.000000
            ZN          N           4.950000
            REST        N          75.000000

S7          Flowrate    M           0.6600    10.0000 %
            CU          M           0.510000  2.00000E-2
            ZN          M          52.100000    2.000000
            REST        N          50.000000

S8          Flowrate    N           0.3500
            CU          M          21.600000    1.000000
            ZN          M           2.100000    2.000000
            REST        N          96.000000
```

The data input is thus finished. The results of the data reconciliation are following (abbreviated):

```
G L O B A L   D A T A

  Mean residue of equations              2.4463E-11
  Qmin                                   3.9550E+00
  Qcrit                                  1.2584E+01
  Status (Qmin/Qcrit)                      0.314289

  S T R E A M S    [T/H],  [%]
  Stream name:  S1
  From node 'ENVIRON' to node 'CELL'

  No. Name       Type       Inp.value       Rec.value       Abs.error
      Flowrate   NO             9.000           9.714           0.673
   1  CU         MC             5.210           5.210           0.020
   2  ZN         MC             5.410           5.410           0.020
   3  REST       NO            95.000          89.380           0.028

  Stream name:  S2
  From node 'CELL' to node 'CUFLOT'

  No. Name       Type       Inp.value       Rec.value       Abs.error
  -------------------------------------------------------------------
      Flowrate   NO             8.000           7.429           0.593
   1  CU         MC             0.450           0.453           0.050
   2  ZN         MC             4.920           4.983           0.126
   3  REST       NO            95.000          94.564           0.134

  Stream name:  S3
  From node 'CUFLOT' to node 'ZNFLOT'

  No. Name       Type       Inp.value       Rec.value       Abs.error
  -------------------------------------------------------------------
      Flowrate   NO             7.000           7.316           0.583
   1  CU         MC             0.130           0.128         8.53E-3
   2  ZN         MC             5.120           5.035           0.128
   3  REST       NO            95.000          94.837           0.129
```

4.10 *Reaction invariant chemical reactor – Burning of a coal*

In the previous examples, chemical reactors were defined by sets of chemical reactions (see also the Section 2.3.3). In some situations, the balance of a chemical reactor can be more conveniently expressed in terms of conservation of elements as the so-called *Reaction invariant reactor.* The theory is described in the Appendix 9. This method requires the knowledge of chemical composition of all species taking part in a chemical conversion.

Let's imagine a coal fired boiler. A coal is burned in contact with the oxygen present in the air. The following species take part in this chemical reaction:

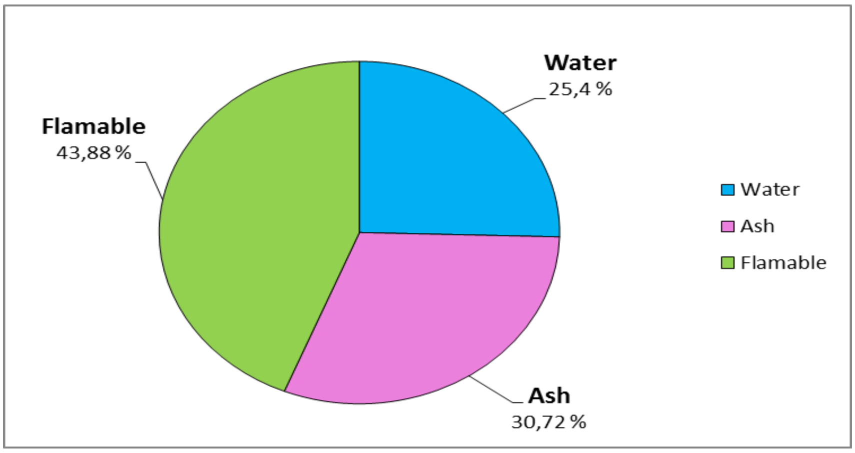
Starting materials are

1. Coal defined by its elemental composition
2. Oxygen (O_2) present in the air

Products are

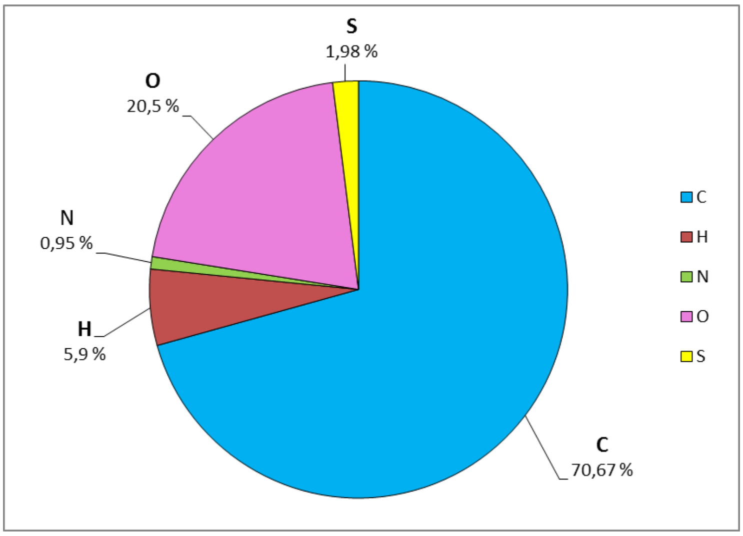
3. Carbon dioxide CO_2
4. Carbon monoxide CO
5. Water (H_2O)
6. Sulphur dioxide (SO_2)
7. Ash, (CO_2)

The coal composition (in this example a typical soft coal) is expressed as a mixture of three parts:



- Moisture (liquid water)
- Ash (hypothetical element comprising a mineral part of a coal)
- Flammable part consisting of carbon, hydrogen, oxygen, nitrogen and sulphur).

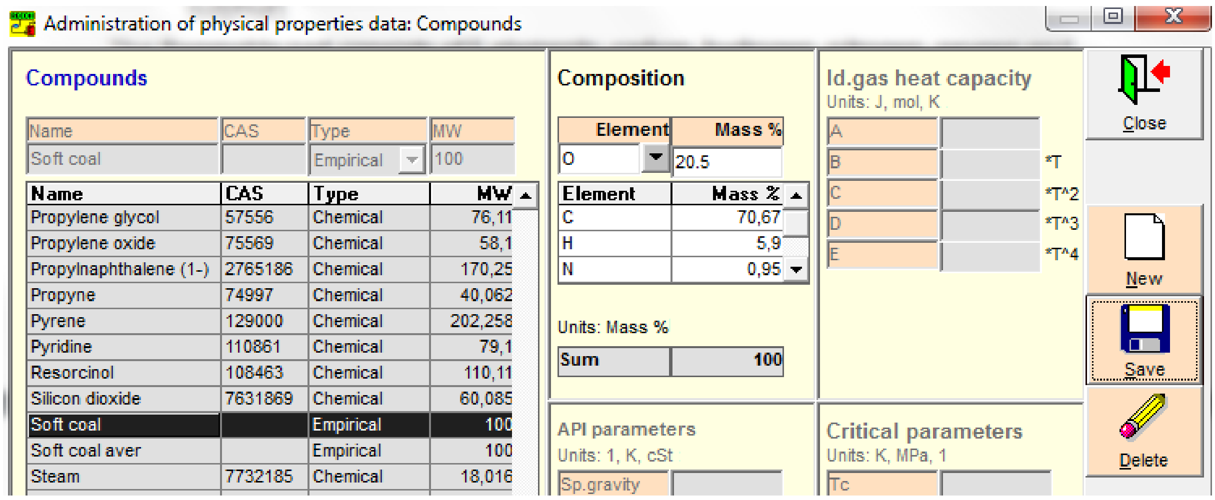
The flammable part consists of 5 elements: carbon, hydrogen, nitrogen, oxygen and sulphur.



Again, this ratio of elements holds for one type of a soft coal.

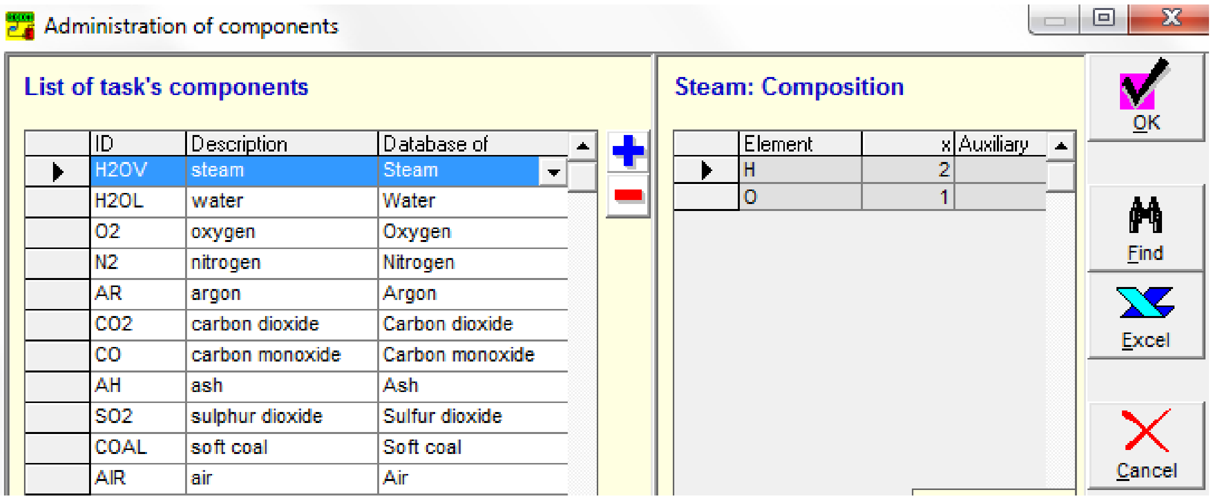
Aside of chemically reacting species there are also non-reacting species, namely nitrogen and rare gases (denoted as Argonne) stemming from the air. In this example we neglect nitrogen oxides which are formed in a very small extent during combustion.

In practice it is convenient to define the flammable part of the coal as a pseudocomponent. The definition of new component which requires administrator's rights is done in the administration part of Recon (*Administration, Physical properties data: Compounds*).



For the compound named *Soft coal* you must enter mass % of elements. The molecular weight of this pseudocomponent is 100. Now we can create the model of coal burning.

Now it is possible to create the model (the DEMO example MC-9). Worth mentioning is the definition of components on the following panel:



It is important to realize that in the list of components only the first two columns are arbitrary and depends on user's choice. The items in the 3rd column must be selected from the database of chemical elements, compounds and mixtures available in Recon. This is because the chemically invariant reactor needs the information on elemental composition of individual components. Note that we have used the component *Soft coal* and the mixture *Air* (to avoid the manual entering of air composition).

The model of the coal firebox can look like this:

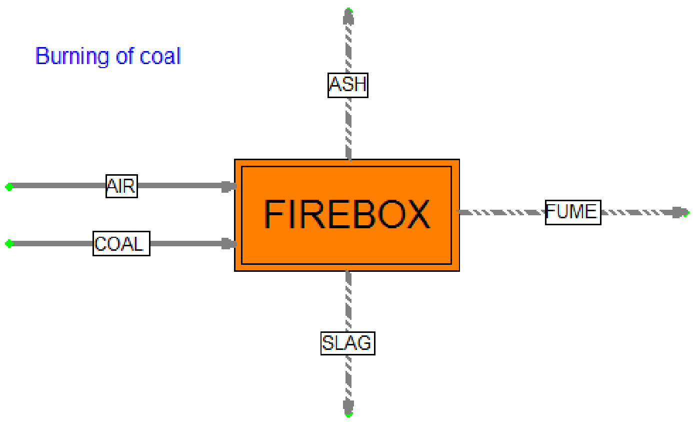


Fig. 4.10-1: Balance flow-sheet (demo example MC-10)

The flows of inputs to the firebox are measured. The compositions of air and coal are fixed. The FUME stream represents gaseous part of flue gases, the mineral part of the coal is divided among the slag leaving the firebox immediately and the flying ash leaving the firebox with flue gases. From the previous measurement it is known that the slug : flying ash ratio is 85 : 15. This ratio is needed to calculate the slug and the flying ash flows. The nonzero variables used in this example are presented in the following table:

Task: MC-9 (Coal firebox)

M A T E R I A L   S T R E A M S

ID	Component	Type	Value	Max.error	
AIR	Flowrate	M	5,0000	5,0000%	KG/S
	AIR	F	100,000000		%wt
ASH	Flowrate	N	5,000E-2		KG/S
	AH	F	100,000000		%wt
COAL	Flowrate	M	1,0000	15,0000%	KG/S
	H2OL	F	25,400000		%wt
	AH	F	30,720000		%wt
	COAL	F	43,880000		%wt
FUME	Flowrate	N	6,0000		KG/S
	H2OV	N	10,000000		%wt
	O2	M	5,000000	0,300000	%wt
	N2	N	50,000000		%wt
	AR	N	1,000000		%wt
	CO2	M	19,000000	1,000000	%wt
	CO	M	5,00000E-2	10,000000%	%wt
	SO2	M	0,260000	0,100000	%wt
SLAG	Flowrate	N	0,2000		KG/S
	AH	F	100,000000		%wt

Note that in the FUME stream O_2, CO_2, CO and SO_2 concentrations are measured. For completeness, here is the user defined equation defining the separation of the slag and the flying ash:

User defined equation:

```
ASH        ash ratio                                                  Model

           [S<ASH>]-0.15*([S<ASH>]+[S<SLAG>])
```

The final results of calculation are in the next table (**note that the *Invariant balance* must be checked on the panel of the FIREBOX node during the calculation**):

RECON 11.8.8-Pro [ChemPlant Technology s.r.o.]
Task: E-14 (Combustion of the soft coa)

Balance: [25.09.2019 15:00; 25.09.2019 16:00)

G L O B A L   D A T A

Number of nodes	1
Number of streams	5
Number of components	11
Number of react. nodes	1

C O M P O N E N T S

ID	Description	Chemical name
H2OV	steam	Steam
H2OL	water	Water
O2	oxygen	Oxygen
N2	nitrogen	Nitrogen
AR	argon	Argon
CO2	carbon dioxide	Carbon dioxide
CO	carbon monoxide	Carbon monoxide
AH	ash	Ash
SO2	sulphur dioxide	Sulfur dioxide
COAL	soft coel flammable part	Soft coal
AIR	air	Air

N O D E S

ID	Description	Remark
ENVIRON	Environment	unbalanced
FIREBOX	firebox	

S T R E A M S

ID	From node	To node	Master stream	Description
AIR	ENVIRON	FIREBOX		air
ASH	FIREBOX	ENVIRON		ash
COAL	ENVIRON	FIREBOX		soft coal
FLUEGAS	FIREBOX	ENVIRON		
SLAG	FIREBOX	ENVIRON		slag

M A T E R I A L   S T R E A M S

ID	Component	Type	Value	Max.error	
AIR	Flowrate	M	5.0000	5.0000%	KG/S
	H2OV	F	0.00000E+0		%wt
	H2OL	F	0.00000E+0		%wt
	O2	F	0.00000E+0		%wt
	N2	F	0.00000E+0		%wt
	AR	F	0.00000E+0		%wt
	CO2	F	0.00000E+0		%wt
	CO	F	0.00000E+0		%wt
	AH	F	0.00000E+0		%wt
	SO2	F	0.00000E+0		%wt
	COAL	F	0.00000E+0		%wt
	AIR	F	100.000000		%wt
ASH	Flowrate	N	5.000E-2		KG/S
	H2OV	F	0.00000E+0		%wt
	H2OL	F	0.00000E+0		%wt
	O2	F	0.00000E+0		%wt
	N2	F	0.00000E+0		%wt
	AR	F	0.00000E+0		%wt
	CO2	F	0.00000E+0		%wt
	CO	F	0.00000E+0		%wt
	AH	F	100.000000		%wt
	SO2	F	0.00000E+0		%wt
	COAL	F	0.00000E+0		%wt
	AIR	F	0.00000E+0		%wt
COAL	Flowrate	M	1.0000	15.0000%	KG/S
	H2OV	F	0.00000E+0		%wt
	H2OL	F	25.400000		%wt
	O2	F	0.00000E+0		%wt
	N2	F	0.00000E+0		%wt
	AR	F	0.00000E+0		%wt
	CO2	F	0.00000E+0		%wt
	CO	F	0.00000E+0		%wt
	AH	F	30.720000		%wt
	SO2	F	0.00000E+0		%wt
	COAL	F	43.880000		%wt
	AIR	F	0.00000E+0		%wt
FLUEGAS	Flowrate	N	6.0000		KG/S
	H2OV	N	10.000000		%wt
	H2OL	F	0.00000E+0		%wt
	O2	M	5.000000	0.300000	%wt
	N2	N	50.000000		%wt
	AR	N	1.000000		%wt
	CO2	M	19.000000	1.000000	%wt
	CO	M	5.00000E-2	10.000000%	%wt
	AH	F	0.00000E+0		%wt
	SO2	M	0.260000	0.100000	%wt
	COAL	F	0.00000E+0		%wt
	AIR	F	0.00000E+0		%wt

```
SLAG       Flowrate    N          0.2000               KG/S
           H2OV        F        0.00000E+0             %wt
           H2OL        F        0.00000E+0             %wt
           O2          F        0.00000E+0             %wt
           N2          F        0.00000E+0             %wt
           AR          F        0.00000E+0             %wt
           CO2         F        0.00000E+0             %wt
           CO          F        0.00000E+0             %wt
           AH          F        100.000000             %wt
           SO2         F        0.00000E+0             %wt
           COAL        F        0.00000E+0             %wt
           AIR         F        0.00000E+0             %wt

W E T N E S S E S    [%]

ID         Type           Value   Max.error
-------------------------------------------
steam      F           0.000E+0
water      F           100.0000

U S E R   E Q U A T I O N S

ID         Description                                             Remark
           Programmatic code
--------------------------------------------------------------------------
ASH        ash ratio                                               Model
           [S<ASH>]-0.15*([S<ASH>]+[S<SLAG>])
```

Results show that even in this small flowsheet there are 3 degrees of redundancy, mostly due to measured concentrations in the FUME stream. It should be noted, that in practice CO_2 concentration measurement is not too much common. Also problems are with measurement of the coal flow. This example will be further evolved in the next chapter in connection with heat balancing.