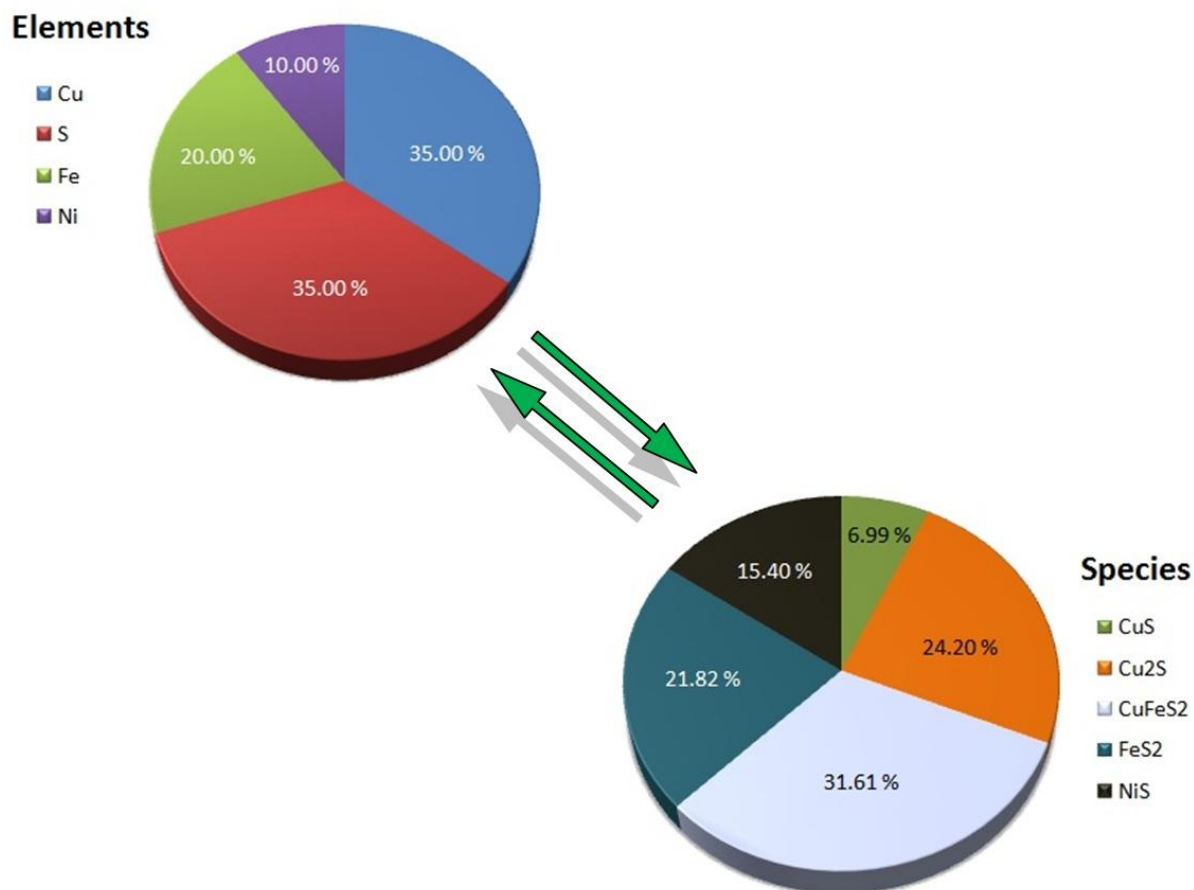# 22. Species Converter Module

SUMMARY

Composition conversions, between substance (mineralogy) and elemental analyses, are often needed in chemical R&D work. The Species Converter module allows you to convert an elemental analysis to a species analysis and vice versa.

You can apply weighting of certain species to increase or decrease their amounts in the converted analysis. Calculations also allow targets to be set on analysis composition to reach a specific weight percentage for selected species. You may also carry out the conversion in ΔG stability order for certain species types.

22.1.   Converting Analyses

To convert elemental analyses to species analyses, first you need to enter the *Input analysis* (**Fig. 1**). Analyses can be typed manually or pasted from e.g. Excel. The species in the analyses do not have to exist in the HSC Database. Please also note that the total wt-% of the input analysis can be below 100%.

	INPUT	
5	**Analysis**	
6		
7	**Elements**	**wt-%**
8	Total	100.000
9	Cu	25.000
10	S	40.000
11	Fe	10.000
12	Ni	25.000
13		

Fig. 1. Enter the Input analysis in the table.

After you have entered the Input analysis, you need to specify the species for the *Output analysis* (**Fig. 2**) and click *Solve* to get the converted analysis (**Fig. 3**). Note that species containing elements which are not present in the input analysis are disregarded in the solution, with the exceptions of oxygen and hydrogen.

OUTPUT	Calculated wt-%	Target wt-%	Weight Coeff	Type
		0.000		
CuS			1.000	
Cu2S			1.000	
CuFeS2			1.000	
FeS2			1.000	
NiS			1.000	
Ni3S2			1.000	

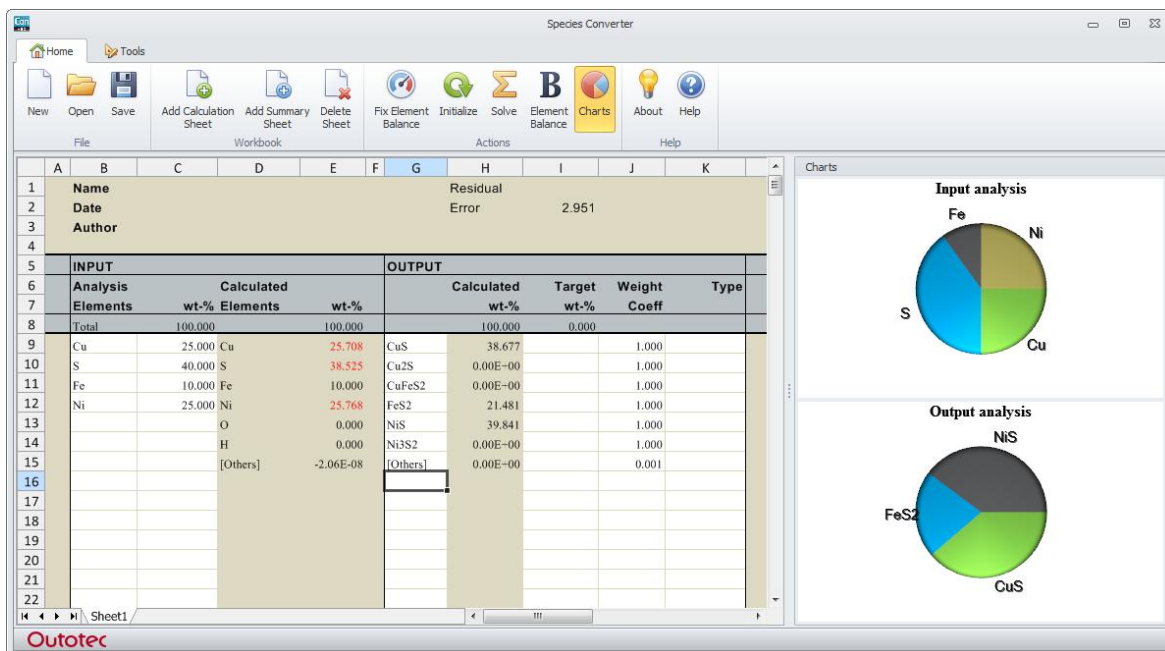**Fig. 2.** Enter the species for the output analysis.

Fig. 3. Converted analysis.

Along with the converted analysis you may get red values in the *Calculated Elements* column if the results failed to reach the input elemental analysis based on the *Limit* set by the user. The default value for the limit is 99.7. This means that the value of the element will be colored red in the Calculated Elements if the ratio of the element amount in the output and input analyses is less than 99.7%[1]. Note that if the element amount in the output analysis is larger than the amount in the input analysis, then the inverse of the ratio is used in the Limit calculation. You can check the calculated Limit value for each element from the *Element Balance* dialog (**Fig. 4**).

$$\frac{N_{e,total}}{N_{e,measured}} * 100 \geq Limit \tag{1}$$

$N_{e,total}$ = Total amount of the element in all of the species in output analysis
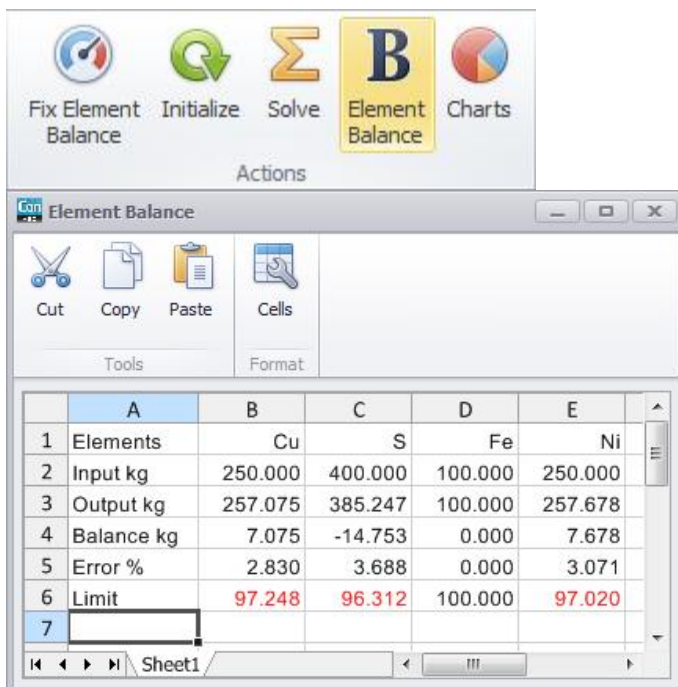$N_{e,measured}$ = Total amount of the element in all of the species in input analysis.

Fig. 4. Element Balance. The Limit values for the elements are red if the values are less than the user-set Limit threshold value.

You can try to resolve Limit failures by modifying the species in the output analysis, or you can add pure elements for elements where the limit failure occurs using *Fix Element Balance* (**Fig. 5**). The added elements will have small weight coefficients by default, so that they do not alter the analysis too much.
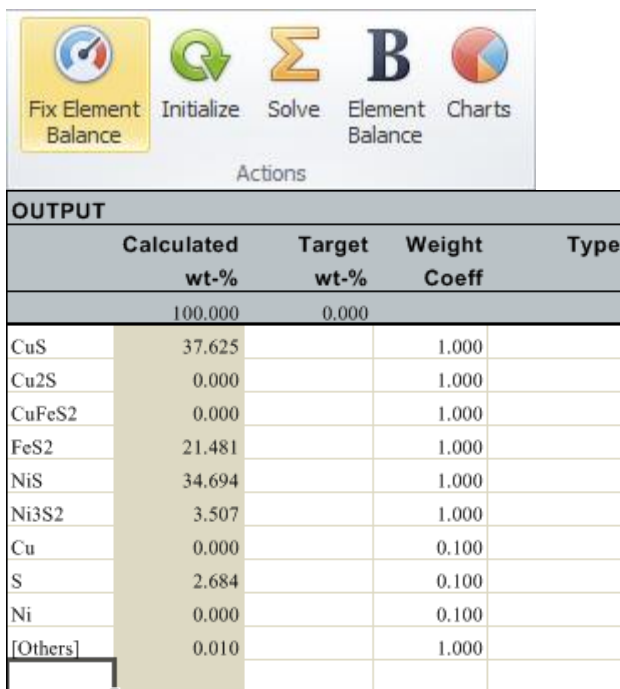

Fig. 5. Fix Element Balance. This will add pure elements to the output analysis to conserve the elemental balance.

Analysis conversion also adds the *[Others]* variable as part of the output analysis. It can be used to include the unknown part of the input analysis. Usually the weight coefficient of this variable is low in order to minimize its amount; however, you can adjust the weight

coefficients at any time to get conversions which better reflect the experimental input analyses. The use of weight coefficients is introduced in *section 22.2 Analysis weighting and Target calculation.*

The *Residual Error* (**Fig. 6**) at the top of the spreadsheet will indicate the "success" of the output analysis solution. The lower the value of the error, the better the solution. The value is calculated using Equation (2).

H	I
Residual Error	0.362

Fig. 6. Residual Error.

$$\text{Residual Error} = \sum \left| N_e - N_{e,measured} \right| \qquad\qquad (2)$$

N_e = Total amount of the element in all the output species
$N_{e,\,measured}$ = Total amount of the element in the input analysis

You can attempt to force the residual error below a set norm value with the *Set norm below the limit* option (**Fig. 7**). You can set the value in the *Norm limit* field and click Solve to get the new conversion with a smaller residual error. Please note that too small norm limits or errors in the analyses can cause the optimization routine to fail and result in a total wt-% exceeding 100%.

Norm limit	0.0001
Set norm below the limit	☑
Norm settings	

Fig. 7. Norm settings can be used to force the residual error below a certain limit. NB! Norm settings can be used only with solution Methods 1 and 2.

The *Exact O and H measurement* options (**Fig. 8**) enable you to specify the amounts of oxygen and hydrogen as the exact amounts entered in the input analysis or as the minimum amounts. If the options are unchecked, you may get an output analysis in which the amount of oxygen or hydrogen is larger than that specified in the input analysis. This can be used, for example, when determining a mineralogical composition for an oxide sample for which the metals compositions are known. If Exact O/H is unchecked, the difference between the measured amount and the calculated amount is not included in the residual error.

☑ Exact O measurement
☑ Exact H measurement
Measurements

Fig. 8. Exact O and H measurement options.

The calculated results can be cleared with the *Initialize* button. Initialization also returns the calculated elemental composition of the input analysis. This is useful, especially in cases where the analysis contains species (**Fig. 9**).

5	**INPUT**				
6	**Analysis**		**Calculated**		
7	**Elements**	**wt-%**	**Elements**		**wt-%**
8	Total	100.000			
9	Cu	25.000	Cu		74.889
10	CuO	25.000	O		15.053
11	Cu2S	25.000	S		10.058
12	CuSO4	25.000			
13					

Fig. 9. The Initialize button will produce the calculated elemental composition of the input analysis.

22.2.   Analysis Weighting and Target Calculation

The output analysis can be adjusted with the use of weighting coefficients. You can easily change the weight coefficient of the species from the *Weight Coeff.* column (**Fig. 2**) and re-calculate the analysis to obtain different results. The greater the weight coefficient of a species is, the greater the amount of included elements will be, in the formation of the species in the output analysis.

You can also set a *Target wt-%* value for a species in the analysis (**Fig. 2**). To use the Target wt-% feature, enter a target value for a selected species and increase the weight coefficient of that species to force the conversion towards the target value.

The three calculation methods available (**Fig. 10**) can provide you with alternative solutions for analysis conversion. These methods differ from each other in terms of how the solution is generated and how they enable the weighting to be applied. The methods are presented briefly in the sections below. The *Small Meas. Limit* value in the same settings (**Fig. 10**) determines the threshold value (wt-%) for the species which are considered as small amounts in the charts.
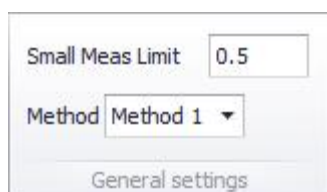
Fig. 10. Calculation methods and the limit for small measurements.

Method 1

Method 1 allows you to apply weight coefficients for species with and without target values. It also enables the use of all the other calculation options. This method requires usually more analysis adjustment (e.g. Fix Element Balance) than the other two methods in order for the solution to reach the element balance limit.

Method 2

Method 2 allows you to apply weight coefficients only for the species that also have a target wt-% value. Weight coefficients without target values will be ignored. This method is a simple least squares method with known target values.

Method 3

Method 3 allows you to apply weight coefficients for species with and without target values to a certain extent. The method requires that the number of species in the output list is greater than the sum of targets and input species, see Equation (3) ([Others] is not considered as a species this case). This method is based on the mathematical method called *Column scaling*. Underdetermined non-negative least squares is used to achieve the solution.

$$N_{\text{Output species}} > N_{\text{Targets}} + N_{\text{Input species}} \qquad\qquad (3)$$

Usually Methods 2 and 3 give a better element balance than Method 1.

22.3.   Stability Weighting

Stability Weighting allows you to form the conversion of specific species types in order of *ΔG* stability. There are currently seven species types that can be used in stability weighting. Only one species type can be selected at a time and the recognized species are indicated in the *Type* column (**Fig. 2**). Note that the species used in Stability Weighting have to exist in the HSC Database, in order for them to have a *ΔG* value.

To form the conversion with *Stability Weighting*, select the correct species type from the top menu drop-down list (**Fig. 11**) and set a weighting coefficient value for the stability weighting. The coefficient works in a similar way to the weight coefficient in the Target calculation, but the weighting is applied to the whole species type. Finally, click Solve to calculate the results.

Species type	Sulfides ▼
Weighting coef.	80

Stability Weighting

OUTPUT

	Calculated wt-%	Target wt-%	Weigh Coeff.	Type
	100.000	0.000		
CuS	3.619		1.000	sulfide
Cu2S	0.000		1.000	sulfide
CuFeS2	55.142		1.000	sulfide
NiS	41.240		1.000	sulfide
Ni3S2	0.000		1.000	sulfide
[Others]	0.000		0.001	
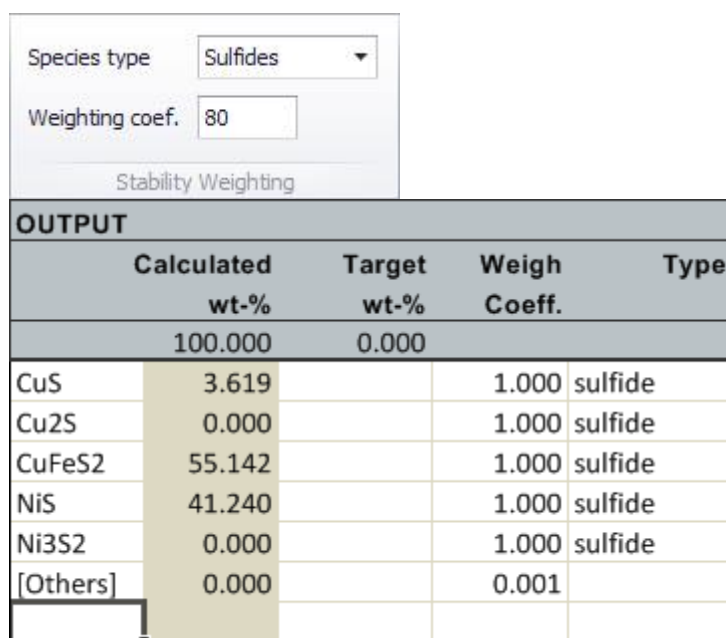
Fig. 11. Stability weighting and species types.

22.4.   Example Conversion

A mineral sample has the elemental composition shown in **Table 1**. In addition, the sample is known to contain sulfide minerals for which the wt-% values are 60% chalcopyrite(CuFeS2), 15% pyrite(FeS2), and 4.5% galena(PbS).

Table 1. Elemental composition of a mineral sample.

Element / Oxide	Wt-%
S	32.850
Cu	25.700
Fe	24.700
Ni	0.550
Co	0.010
Zn	4.050
Pb	3.900
Sb	0.200
As	0.130
Ag	0.090
Au	0.001
SiO2	4.650
Al2O3	2.200
MgO	0.150
Total	99.181

The elemental analysis of the sample can be copied as the input analysis for the conversion. Next, the output analysis needs to be defined with species that are expected to be present in the sample (**Table 2**).

Table 2. Expected mineral species in the sample and their estimated proportions.

Species	Estimated Wt-%
CuS	
Cu2S	
CuFeS2	60.0
FeS	
FeS2	15.0
NiS	
CoS	
ZnS	
PbS	4.5
Sb2S3	
As2S3	
Ag2S	
Au	
SiO2	
Al2O3	
MgO	

To promote the target values in the solution, the weight coefficient of three species can be increased to 10.0 (**Fig. 12**).

INPUT				OUTPUT			
Analysis		Calculated			Calculated	Target	Weight	Type
Elements	wt-%	Elements	wt-%		wt-%	wt-%	Coeff	
Total	99.181					79.500		
S	32.850			CuS			1.000	
Cu	25.700			Cu2S			1.000	
Fe	24.700			CuFeS2		60.000	10.000	
Ni	0.550			FeS			1.000	
Co	0.010			FeS2		15.000	10.000	
Zn	4.050			NiS			1.000	
Pb	3.900			CoS			1.000	
Sb	0.200			ZnS			1.000	
As	0.130			PbS		4.500	10.000	
Ag	0.090			Sb2S3			1.000	
Au	1.00E-03			As2S3			1.000	
SiO2	4.650			Ag2S			1.000	
Al2O3	2.200			Au			1.000	
MgO	0.150			SiO2			1.000	
				Al2O3			1.000	
				MgO			1.000	

Fig. 12. Defined input and output analyses. Weight coefficients of the target values have been increased to 10.0.

A solution calculated with Method 1 for the output analysis is shown in **Fig. 13**.

Name	Example Conversion			Residual				
Date				Error	1.076			
Author								

INPUT				OUTPUT			
Analysis		Calculated			Calculated	Target	Weight	Type
Elements	wt-%	Elements	wt-%		wt-%	wt-%	Coeff	
Total	99.181		100.000		100.000	79.500		
S	32.850	S	33.259	CuS	0.00E+00		1.000	
Cu	25.700	Cu	25.571	Cu2S	6.006		1.000	
Fe	24.700	Fe	25.239	CuFeS2	59.997	60.000	10.000	
Ni	0.550	Ni	0.550	FeS	0.00E+00		1.000	
Co	0.010	Co	0.010	FeS2	14.995	15.000	10.000	
Zn	4.050	Zn	4.050	NiS	0.850		1.000	
Pb	3.900	Pb	3.900	CoS	0.015		1.000	
Sb	0.200	Sb	0.200	ZnS	6.036		1.000	
As	0.130	As	0.130	PbS	4.503	4.500	10.000	
Ag	0.090	Ag	0.090	Sb2S3	0.279		1.000	
Au	1.00E-03	Au	1.00E-03	As2S3	0.213		1.000	
SiO2	4.650	Si	2.174	Ag2S	0.103		1.000	
Al2O3	2.200	Al	1.164	Au	1.00E-03		1.000	
MgO	0.150	Mg	0.090	SiO2	4.650		1.000	
		O	3.572	Al2O3	2.200		1.000	
		H	0.000	MgO	0.150		1.000	
		[Others]	-1.98E-08	[Others]	0.00E+00		0.001	

Fig. 13. Conversion results. Please note that the element balance limit is not reached for sulfur, copper, and iron.

If the results from **Fig. 13** are compared with the results calculated with Method 2 (**Fig. 14**), it can be seen that Method 2 produces a better elemental balance and a smaller Residual Error in this particular example. However, this comparison also shows that the calculated values are closer to the given target values for the results calculated with Method 1. (*Note that Method 3 cannot be used in this example because the amount of input species (14) + target values (3) is equal to the amount of output species (17)*).

Name	Example Conversion				Residual				
Date					Error	0.017			
Author									
INPUT				**OUTPUT**					
Analysis		Calculated			Calculated	Target	Weight		Type
Elements	wt-%	Elements	wt-%		wt-%	wt-%	Coeff		
Total	99.181		100.000		100.000	79.500			
S	32.850	S	32.850	CuS	0.676				
Cu	25.700	Cu	25.700	Cu2S	5.827				
Fe	24.700	Fe	24.717	CuFeS2	59.483	60.000	10.000		
Ni	0.550	Ni	0.550	FeS	0.00E+00				
Co	0.010	Co	0.010	FeS2	14.210	15.000	10.000		
Zn	4.050	Zn	4.050	NiS	0.850				
Pb	3.900	Pb	3.900	CoS	0.015				
Sb	0.200	Sb	0.200	ZnS	6.036				
As	0.130	As	0.130	PbS	4.503	4.500	10.000		
Ag	0.090	Ag	0.090	Sb2S3	0.279				
Au	1.00E-03	Au	1.00E-03	As2S3	0.213				
SiO2	4.650	Si	2.174	Ag2S	0.103				
Al2O3	2.200	Al	1.164	Au	1.00E-03				
MgO	0.150	Mg	0.090	SiO2	4.650				
		O	3.572	Al2O3	2.200				
		H	0.000	MgO	0.150				
		[Others]	0.802	[Others]	0.802				

Fig. 14. Conversion results calculated with Method 2.

22.5.   Description of the Conversion Methods

Abbreviations

N_E number of measured elements excluding oxygen and/or hydrogen

N_C number of compounds to be calculated

pE_i measured percentage of the i th element

$(AM)_i$ atomic mass of the i th element

M_i molecular mass of the i th calculated compound

M_i^M molecular mass of the i th measured compound

$C_{i,j}$ coefficient of the i th element in the j th calculated compound (e.g. if the i th element is S and the j th compound is CuFeS2, then the coefficient is 2)

$C_{i,j}^M$ coefficient of the i th measured compound in the j th compound (e.g. if the i th measured compound is H2O and the j th compound is CaSO4*2H2O, then this coefficient is 2. If the i th measured compound is Fe3O4 and the j th compound is Fe3O4, then this coefficient is 1)

$C_{O,j}$ coefficient of oxygen in the j th compound

$C_{H,j}$ coefficient of hydrogen in the j th compound

$(AM)_O$ atomic mass of oxygen

$(AM)_H$ atomic mass of hydrogen

p_j calculated amount of the j th compound

N_{CS} number of compounds given in stability order e.g. number of oxides, sulfates, sulfides, carbonates, chlorides or fluorides

T_j target value of the j th compound

1. Calculation of percentages of compounds from the element measurements

Compound measurements may exist. All measured compounds such as oxides (SiO, Al2O3, MgO, CaO,..) are converted back to elements (Si, Al, Mg, Ca, O,…) before the calculation starts.

There are three methods to solve the problem:

Method 1

The mass balance equations for the elements are

$$i = 1,...,N_E$$

$$\sum_{j=1}^{N_C} \frac{C_{i,j}(AM)_i}{M_j} p_j = pE_i$$

Let matrix B be

$$B_{i,j} = L_i \frac{C_{i,j}(AM)_i}{M_j}$$

$$i = 1,...,N_E$$
$$j = 1,...,N_C$$

and vector b be

$$b_i = L_i pE_i$$
$$i = 1,...,N_E$$

Where

$$L_i = 10000 \quad if \ pE_i < 15$$

$$L_i = 1 \quad otherwise$$

Now the mass balance equations can be written in matrix form:

$$Bp = b$$

It is possible, although not very common, that oxygen and/or hydrogen measurements exist. The measured amounts of these elements can be set as minimum amounts or exact amounts. If the amount of oxygen/hydrogen is considered as an exact amount, N_E also contains oxygen/hydrogen.

If the measured amounts of oxygen and hydrogen are considered as minimum amounts, the equations for oxygen and/or hydrogen are

$$\sum_{j=1}^{N_C} \frac{C_{O,j}(AM)_O}{M_j} p_j \geq pE_O$$

$$\sum_{j=1}^{N_C} \frac{C_{H,j}(AM)_H}{M_j} p_j \geq pE_H$$

Let matrix E be

$$E_{1,j} = \frac{C_{O,j}(AM)_O}{M_j}$$

$$E_{2,j} = \frac{C_{H,j}(AM)_H}{M_j}$$

and vector f be

$$f_1 = pE_O$$
$$f_2 = pE_H$$

If oxygen and/or hydrogen are not measured, the corresponding row(s) of matrix E and vector f are omitted. If O and H measurements are considered as exact amounts, they are treated as other elements and matrix E and vector f are omitted.

Each compound has a given weight w_{ii}. Let W be the N_C x N_C diagonal matrix of the weights. The greater the weight w_{ii}, the more we try to create the i th compound. The default value of a weight is 1.

We might have some known target values for compounds. Usually these target values come from mineralogical analysis. Let diagonal matrix D be

$$D_{i,i} = \begin{cases} w_{ii} & \text{if } T_i \text{ is given} \\ 0 & \text{if } T_i \text{ is not given} \end{cases}$$

$$D_{i,j} = 0 \quad i \neq j$$

and vector d

$$d_i = \begin{cases} w_{ii}T_i & \text{if } T_i \text{ is given} \\ 0 & \text{if } T_i \text{ is not given} \end{cases}$$

Now we have to solve the following problem:

$$\min\|Hp - h\|_2^2 \text{ subject to } p \geq 0 \text{ and } Ep \geq f$$

$$\text{where } H = \begin{vmatrix} W^{-1} \\ 100*B \\ 10000*D \\ 100000....100000 \end{vmatrix} \text{ and } h = \begin{vmatrix} 0 \\ 100*b \\ 10000*d \\ 100000*100 \end{vmatrix}$$

The condition $[100000...100000]p = 100000*100$
guarantees that the sum of the percentages of the compounds is 100.

Method 2

The mass balance equations for the elements are

$$i = 1,...,N_E$$
$$\sum_{j=1}^{N_C} \frac{C_{i,j}(AM)_i}{M_j}p_j = pE_i$$

Let matrix B be

$$B_{i,j} = L_i \frac{C_{i,j}(AM)_i}{M_j}$$
$$i = 1,...,N_E$$
$$j = 1,...,N_C$$

and vector b be

$$b_i = L_i pE_i$$
$$i = 1,...,N_E$$

Where

$$L_i = 10000 \quad \textit{if } pE_i < 15$$

$$L_i = 1 \quad \textit{otherwise}$$

Now we can write the mass balance equations in matrix form:

$$Bp = b$$

It is possible, although not very common, that oxygen and/or hydrogen measurements exist. The measured amounts of these elements can be set as minimum amounts or exact amounts.

If the measured amounts of oxygen and hydrogen are considered as minimum amounts, the equations for oxygen and/or hydrogen are

$$\sum_{j=1}^{N_C} \frac{C_{O,j}(AM)_O}{M_j} p_j \geq pE_O$$

$$\sum_{j=1}^{N_C} \frac{C_{H,j}(AM)_H}{M_j} p_j \geq pE_H$$

Let matrix E be

$$E_{1,j} = \frac{C_{O,j}(AM)_O}{M_j}$$

$$E_{2,j} = \frac{C_{H,j}(AM)_H}{M_j}$$

and vector f be

$$f_1 = pE_O$$
$$f_2 = pE_H$$

If oxygen and/or hydrogen are not measured, the corresponding row(s) of matrix E and vector f are omitted. If O and H measurements are considered as exact amounts, they are treated as other elements and matrix E and vector f are omitted.

We might have some known target values for compounds. Usually these target values come from mineralogical analysis. Each compound with a given target value has a given weight w_{ii}. Let diagonal matrix D be

$$D_{i,i} = \begin{cases} w_{ii} & \text{if } T_i \text{ is given} \\ 0 & \text{if } T_i \text{ is not given} \end{cases}$$

$$D_{i,j} = 0 \quad i \neq j$$

and vector d

$$d_i = \begin{cases} w_{ii}T_i & \text{if } T_i \text{ is given} \\ 0 & \text{if } T_i \text{ is not given} \end{cases}$$

Now we have to solve the following problem:

$$\min\|Hp - h\|_2^2 \text{ subject to } p \geq 0 \text{ and } Ep \geq f$$

$$\text{where } H = \begin{vmatrix} 100 * B \\ 10000 * D \\ 100000....100000 \end{vmatrix} \text{ and } h = \begin{vmatrix} 100 * b \\ 10000 * d \\ 100000 * 100 \end{vmatrix}$$

The condition $\begin{bmatrix} 100000...100000 \end{bmatrix} p = 100000 * 100$
guarantees that the sum of the percentages of the compounds is 100.

Method 3

Each compound has a given weight w_j. Let W be a diagonal matrix defined as

$$W_{ii} = \begin{cases} w_i & \text{if compound i has no target value} \\ 1 & \text{if target value exists} \end{cases}$$

The mass balance equations for the elements are

$$i = 1,...,N_E$$
$$\sum_{j=1}^{N_C} \frac{C_{i,j}(AM)_i}{M_j} p_j = pE_i$$

Let matrix B be

$$B_{i,j} = W_i \frac{C_{i,j}(AM)_i}{M_j}$$

$$i = 1,...,N_E$$

$$j = 1,...,N_C$$

and vector b be

$$b_i = pE_i$$

$$i = 1,...,N_E$$

Now we can write the mass balance equations in matrix form:

$$Bp = b$$

It is possible, although not very common, that oxygen and/or hydrogen measurements exist. The measured amounts of these elements can be set as minimum amounts or exact amounts.

If the measured amounts of oxygen and hydrogen are considered as minimum amounts, the equations for oxygen and/or hydrogen are

$$\sum_{j=1}^{N_C} \frac{C_{O,j}(AM)_O}{M_j} p_j \geq pE_O$$

$$\sum_{j=1}^{N_C} \frac{C_{H,j}(AM)_H}{M_j} p_j \geq pE_H$$

Let matrix E be

$$E_{1,j} = W \frac{C_{O,j}(AM)_O}{M_j}$$

$$E_{2,j} = W \frac{C_{H,j}(AM)_H}{M_j}$$

and vector f be

$$f_1 = pE_O$$
$$f_2 = pE_H$$

If oxygen and/or hydrogen are not measured, the corresponding row(s) of matrix E and vector f are omitted. If O and H measurements are considered as exact amounts, they are treated as other elements and matrix E and the vector f are omitted.

We might have some known target values for compounds. Usually these target values come from mineralogical analysis. Let matrix D be

$$D_{i,i} = \begin{array}{l} w_{ii} * 0.001 \quad if \quad T_i \quad is \quad given \\ \\ 0 \quad if \quad T_i \quad is \quad not \quad given \end{array}$$

$$D_{i,j} = 0 \quad i \neq j$$

and vector d

$$d_i = \begin{array}{l} w_{ii} * 0.001 * T_i \quad if \quad T_i \quad is \quad given \\ \\ 0 \quad if \quad T_i \quad is \quad not \quad given \end{array}$$

Now we have to solve the following problem:

$$\min \lVert Hp - h \rVert_2^2 \text{ subject to } p \geq 0 \text{ and } Ep \geq f$$

where $H = \begin{vmatrix} B \\ D \\ 1....1 \end{vmatrix}$ and $h = \begin{vmatrix} b \\ d \\ 100 \end{vmatrix}$

The solution is

$$p = Wp$$

2. Calculation of compounds in order of stability

Stability order calculations are only available if Method 1 or Method 2 is selected.

Let the stability order of sulfates, sulfides, carbonates, fluorides and chlorides be given. First we create the chosen type of compound in order of stability until all elements are consumed or the amount of compounds exceeds 100%. We now suppose that the number of compounds N_C contains the compounds created in order of stability.

Let pS be the vector of amounts of sulfides, sulfates, carbonates, fluorides or chlorides created in order of stability. Now we can form the mass balance equations as follows:

$$\min \lVert Hp - h \rVert_2^2 \text{ subject to } p \geq 0.$$

Method 1

where $H = \begin{vmatrix} W^{-1} \\ 100 * B \\ 100000..100000 \\ \lambda * S \end{vmatrix}$ and $h = \begin{vmatrix} 0 \\ 100 * b \\ 100000 * 100 \\ \lambda * pS \end{vmatrix}$

Method 2

$$\text{where } H = \begin{vmatrix} 100*B \\ 100000...100000 \\ \lambda*S \end{vmatrix} \text{ and } h = \begin{vmatrix} 100*b \\ 100000*100 \\ \lambda*pS \end{vmatrix}$$

B and W as above and

$$S_{ij} = \begin{cases} 0, & ith \;\; compound \;\; in \;\; stability \;\; order \neq jth \;\; compound \\ 1, & ith \;\; compound \;\; in \;\; stability \;\; order = jth \;\; compound \end{cases}$$

$$i = 1,...,N_{CS}, \; j = 1,...,N_C$$

The number λ may be varied according to how much weight we want to give to the values of vector pS.

3. Constrained residual norm

It is also possible to solve the following problem for Methods 1 and 2:

$$\min \left\| W^1 p \right\|_1 \text{ subject to } \left\| Bp - b \right\|_2 \leq \varepsilon \text{ and}$$

$$[1...1]p = 100 \text{ and } p \geq 0$$

This problem is known as weighted non-negative basis pursuit denoising and is described in more detail in[3-4].

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22.6.   References

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