7. Chemical Calculation

7.2 Conversion of measurement values (per litre) into the concentration in the environmental sample (per kg)

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At the ICP-OES, the P concentration per litre in the sample solution is automatically calculated from the measured element-typical light intensity with the help of the previously measured and automatically calculated calibration line. Regarding the molybdenum blue method concentrations of P per litre solutions are calculated as well. Normally, concentrations of P are presented in µg or mg per litre. In the following example for calculation the P concentration in mg l^{-1} is converted into mg kg^{-1}. For all other units the procedure is analogous. In any case the units of the weigh-in and of the extract volume also have to be considered. Before converting the P concentration of sample per litre in P concentration per kg, the blanks have to be subtracted. The extract volume is either the added extracting agent volume (if not filled to defined volume after extraction) or that volume, to which the extract was filled after extraction. It is <u>not</u> the subvolume, which is taken for measurement of the analyte.

List of given and searched variables

<u>Example</u>

given:

digestion of a soil sample with *aqua regia*
weigh-in: 0.500 g
Extraction agent: 6 ml conc. HCl + 2 ml conc. HNO_3
Extract volume (filled after digestion): 100 ml
Concentration of analyte in mg P l^{-1} example: 2.635 mg P l^{-1}

searched:

concentration of analyte in mg P per kg material

Approach to find the equation

1. question: Which amount of the analyte is in the extract volume?

This is calculated by a ratio equation from concentration of the analyte in the extract and the extract volume. Since the extract volume is given in ml, the concentration is also calculated in ml.

given:

concentration: x mg P per 10^3 ml — e.g.: 2.635 mg P 10^{-3} ml^{-1}

extract volume: a ml — 100 ml

searched:

mg P per extract volume: y_1

ratio equation:

$$\frac{x \text{ mg}}{10^3 \text{ ml}} = \frac{y_1 \text{ mg}}{a \text{ ml}} \qquad \text{e.g.} \quad \frac{2.635 \text{ mg P}}{10^3 \text{ ml}} = \frac{y_1 \text{ mg}}{100 \text{ ml}}$$

Conversion of equation to y_1 mg means:

$$\frac{x \text{ mg} \times a \text{ ml}}{10^3 \text{ ml}} = y_1 \text{ mg} \qquad \text{e. g.} \quad \frac{2.635 \text{ mg P} \times 100 \text{ ml}}{10^3 \text{ ml}} = 0.2635 \text{ mg P}$$

In our example 0.2635 mg P are in 100 ml. Since the complete P of the weigh-in material is in this extract volume (100 ml), the P in the extract volume is equivalent to the P of the weigh-in. Therefore, 0.2635 mg P are in 0.5 g soil.

2. question: If y_1 mg P are in the weigh-in of the materials, how many mg P are in 1 kg of the material?

This is calculated by a ratio equation as well. It has to considered that the weigh-in is in g and the mass reference of the material is in kg. For this reason, it is calculated with 10^3 g (instead of 1 kg) for the material.

given:

y_1 mg P in b g weigh-in — e.g.: 0.2635 mg P in 0.5 g soil

searched:

y_2 mg P in 10^3 g material

ratio equation:

$$\frac{y_1 \text{ mg}}{\text{b g weigh-in}} = \frac{y_2 \text{ mg}}{10^3 \text{ g material}} \qquad \text{e.g.: } \frac{0.2635 \text{ mg P}}{0.5 \text{ g weigh-in}} = \frac{y_2 \text{ mg}}{10^3 \text{ g soil}}$$

Converting the equation to y_2 mg means:

$$\frac{10^3 \text{ g} \times y_1 \text{ mg}}{\text{b g weigh-in}} = y_2 \text{ mg} \qquad \text{e.g.: } \frac{10^3 \text{ g} \times 0.2635 \text{ mg P}}{0.5 \text{ g weigh-in}} = 527 \text{ mg P}$$

In our example the soil has a P concentration of 527 mg kg^{-1}.

To calculate not always stepwise, the formula converted to y_1 can be inserted for y_1 in the formula converted to y_2.

The formula $$\frac{\text{x mg} \times \text{a ml}}{10^3 \text{ ml}} = y_1 \text{ mg}$$

is inserted in the formula $$\frac{10^3 \text{ g} \times y_1 \text{ mg}}{\text{b g weigh-in}} = y_2 \text{ mg}$$

instead of y_1. This results in the following formula:

$$\frac{10^3 \text{ g} \times \text{x mg} \times \text{a ml extract volume}}{10^3 \text{ ml} \times \text{b g weigh-in}} = y_2 \text{ mg P kg}^{-1} \text{ material}$$

Both 10^3 cancel each other. If P concentration is measured in (mg) per litre, the weigh-in is given in g and the extract volume in ml, the P concentration in the environmental sample in (mg) per kg material can be calculated by the following formula:

$$\frac{\text{x mg} \times \text{a ml extract volume}}{\text{b g weigh-in}} = y_2 \text{ mg P kg}^{-1} \text{ material}$$

This means for our example:

$$\frac{2.635 \text{ mg P} \times 100 \text{ ml extract volume}}{0.5 \text{ g soil}} = 527 \text{ mg P kg}^{-1} \text{ soil}$$

If the extract was diluted, the dilution factor (DF) has to be considered. This factor has to be inserted as multiplier in the formula, since without dilution the concentration in the extract would have been higher.

$$\frac{\text{x mg} \times \text{a ml extract volume} \times \text{DF}}{\text{b g weigh-in}} = y_2 \text{ mg P kg}^{-1} \text{ material}$$

If in our example one part of the soil extract would have been diluted (= mixed) with one part of water, the DF would be 2. If one part of the soil extract would have been diluted (= mixed) with two parts of water, the DF would be 3.
The P concentration of 527 mg P per kg soil would be therefore 1054 mg P with DF 2 and for DF 3 1581 mg per kg soil. More information about dilution and mixture can be found in the chapter 7.1 Dilution and mixtures.

In an excel sheet the order of columns could be as follows. If further elements were determined by ICP-OES, the columns for other elements have to be added.

Table 7.2-1 Order of columns for calculation of P concentration in an environmental sample from OCP-OES measurement of P-concentration

Columns	Content of columns
A	Identification(number) of sample
B	Measurement value of ICP-OES, e.g. mg P per litre
C	extract volume in ml
D	Weigh-in in g
E	Dilution factor
F	Mean of blank values, e.g. in mg P per litre
G	Measured value minus mean of blanks
H	Calculation of P concentration in the environmental sample with the following formula: column G * column C * column E / column D
I	If necessary, further conversion of the P concentration, e.g. from mg per kg in g per kg or mol per kg

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