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EASYCAL

Modules

Innovation with Integrity

Handheld XRF

Table of Contents

1. Introduction

Glossary:	A module is a value that is computed from the concentration of measured compounds or from other modules.

The computation uses one of the following formulae

$$Mod = \frac{K + \sum_i \lambda_i \cdot C_i}{K' + \sum_j \lambda_j \cdot C_j} \qquad \text{or} \qquad Mod = \left(K + \sum_i \lambda_i \cdot C_i \right) \left(K' + \sum_j \lambda_j \cdot C_j \right)$$

in which Mod is the module

λ_i, λ_j, K and K' are constants

C_i and C_j represent the concentration of measured compounds or other modules.

The MODULES program is aimed at defining modules and storing them in a MLB file. When performing an automatic evaluation after the measurement (with the program QUANTEVL), the evaluation program computes the modules only if one of the following conditions is fulfilled:

- the name of the MLB file in which the modules to be calculated are stored is the same as the measurement method (MM file), and the MLB file is located in the directory default directory, usually `C:\SPECEdx\Libraries\MeasMethods\`, or
- the MLB file was declared in an evaluation model (EVM file generated by APPLICATIONSETUP or EVAL) that has the same name as the measurement method (MM file).

As the results is printed through a mapping (WZM file created by QUERYRES/Results Manager), you have to indicate in the mapping to print out modules. It is done by:

- selecting the MLB file: in the **Modules/Input/Database** tab, click on the **Import Module** button, and browse to the MLB file in the Choose a Modules Library dialog box;
- including the modules in the formatting: in the **Modules** text box, select the module and click on the **Add to output** button.

When performing an interactive evaluation with EVAL, the evaluation program computes the modules only if one of the following conditions is fulfilled:

- the MLB file was declared to EVAL, or
- the MLB file was declared in the evaluation model (EVM file generated by APPLICATIONSETUP or EVAL) that was defined while importing the data.

2. Starting MODULES

You can start MODULES from:

- The **SPECTRA EDX Launcher**.

  1. Click the **Tools** button to display the related menu.
  2. Click **Module Editor**

- The Windows Explorer or My Computer:

You can start MODULE by clicking on a **MLB file** icon; this file is then automatically opened in MODULES.

3. Managing MLB Files

In MODULES, you can:

- Create a new file

  On the toolbar, click on the **New** button: MODULES displays an empty file.

New button

- Open an existing MLB file

  On the toolbar, click on the **Open** button, display the folder containing the MLB files, and then double-click the MLB file of your choice to open it.

Open button

- Save a MLB file

  On the toolbar, click on the **Save** button. If you're saving for the first time, MODULES prompts you to name the document. Keep in mind that MLB files must be saved in the directory corresponding to the value of the **`User Calculation Methods Path`** subkey of the **`HKEY_CURRENT_USER\Software\Socabim\Spectra plus S2\`** key in the Windows registry (by default: `C:\Spectra EDX\Libraries\MeasMethods\`).

Save button

4. Using Modules

4.1. Creating a New Module

To create a new module, type in the name of the new module in the **Current module for edition** text box, click on the **Insert** button, and then follow the following guidelines for defining it.

4.1.1. Step 1: Define the module

Warning:	When specifying the compounds from which the modules must be computed, use the same mode (Compounds or Elements) as the one used for the evaluation. For instance, if you display the evaluation results as oxides in EVAL, you must specify the compounds during definition of the modules as oxides too.

Example of definition: if the module $A1$ is defined as follows:

$$A1 = \frac{10\% + C_{Al_2O_3} + A0}{5\% + 2 \times C_{MgO}}$$

the corresponding settings are in MODULES:

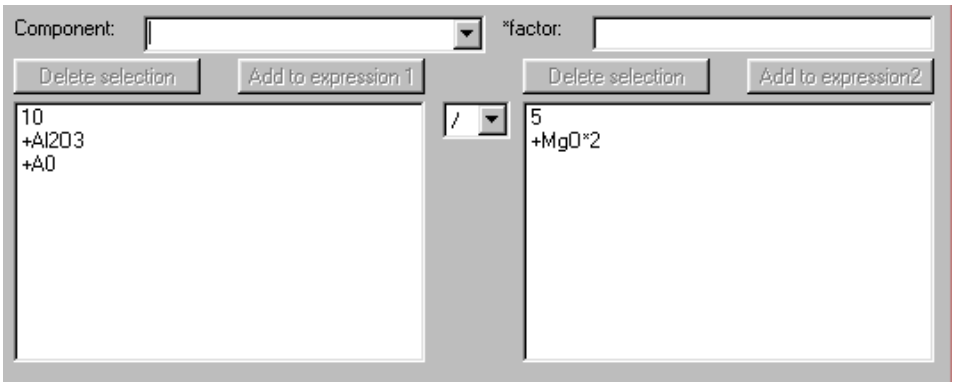

Fig. 4-1 Example of operation

For that, do the following:

1. In the **Component** text box, type in `10`, and then click **Add to expression1**.
2. In the **Component** text box, type in `Al2O3`, and then click **Add to expression1**.
3. In the **Component** text box, type in `A0`, and then click **Add to expression1**.
4. In the list of operations, select "`/`".
5. In the **Component** text box, type in `5`, and then click **Add to expression2**.
6. In the **Component** text box, type in `MgO`, type in `2` in the ***factor** text box, and then click **Add to expression2**.

To delete a component in either the **Numerator** or the **Denominator** list, click it, and then click **Delete selection**.

Reserved names

The names corresponding to calculated concentrations are called "reserved name", which means that they cannot be calculated by a module, their value is picked from the database Measure.MDB. In the example above, `Al2O3` and `MgO` are reserved names.

In fact, it is also possible to use other values like the sum or the loss on ignition (when relevant); these are reserved names too.

You can type the reserved names in the **Component** text box, with the exact spelling, but you can also retrieve them from the files to avoid any error. Three options are available:

Insert Formulas button

- retrieve the chemical formula of the compounds from the calibration file (FCL file): use the menu **Edit | Insert Formulas from calibration...** or the **Insert Formulas** button;

Insert Names button

- retrieve the compound name of the compounds from the calibration file (FCL file): use the menu **Edit | Insert Names from calibration...** or the **Insert Names** button;

Database definitions button

- retrieve the fields of the database that are defined in an Sample Edition Table of the LOADER (DEF file): use the menu **Edit | Insert Database definitions...** or the **Database definitions** button;

The names are then available in the **Component** drop-down list.

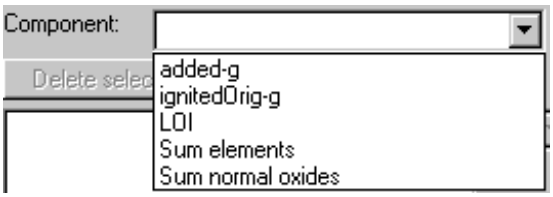

Fig. 4-2 Choice of the reserved names in the drop-down list

Note: if you do not specify a denominator or numerator

In this case, the denominator or numerator is automatically set to 1. For instance, formula

$$A1 = \frac{1}{5\% + 2 * C_{MgO}}$$

corresponds to the following:

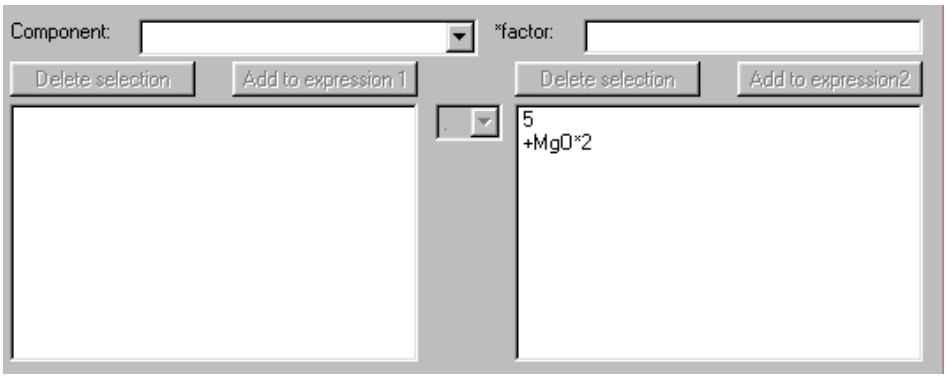

Fig. 4-3 Example of operation with the numerator equal to 1

4.1.2. Step 2: Decide whether the module shall be printed out or not

- Click the **Printable result** option to indicate that the current module shall be printed out.
- Click the **Intermediate step of calculation** to indicate that the current module shall not be printed.
- Set a condition for printing the concentration.
- You can set conditions on the concentration of the current module or/and other compounds and modules for printing out the module.

Warning:	When setting conditions on the concentration of measured compounds, keep in mind that the measured compounds must be specified in the same mode (Calibration compounds, Compounds or Elements) as the one used for the evaluation. For instance, if you display the evaluation results as oxides in EVAL, you must specify the compounds during definition of the modules as oxides too.

Example of condition:

`Print current module (A1) if A1 concentration is greater or equal to 5 AND the concentration of` Na_2O `is lower than 15%.`

This condition is specified the following way in MODULES (keep in mind to select the **Condition** check box before defining the condition):

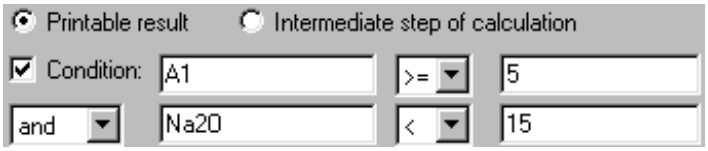

Fig. 4-4 Setting a condition

4.2. Editing Existing Modules

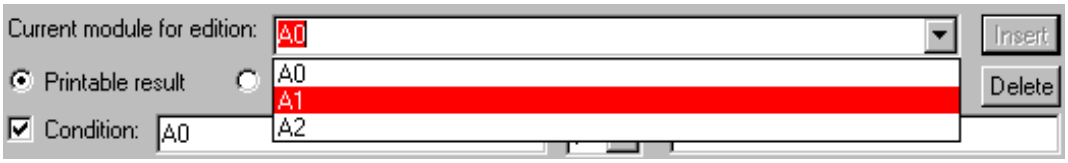

Fig. 4-5 Editing existing modules

You can edit existing modules by selecting the module of interest in the list of existing modules, and then perform changes.

To delete an existing module, select in the list of existing modules, and then click **Delete**. Make sure that the module to be deleted is not taken as a reference in other modules.

5. Printout of Modules

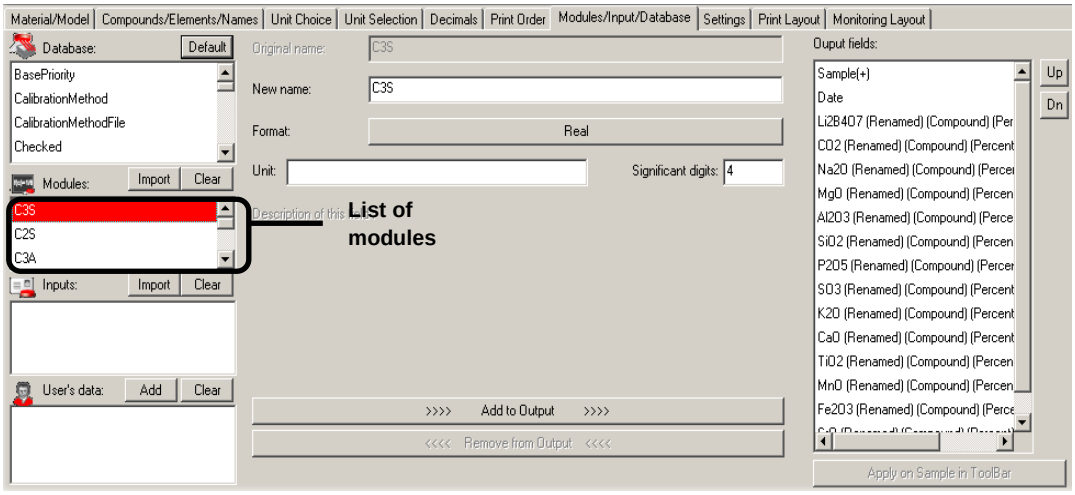

*Fig. 5-1 QueryRes: **Modules/Input/Database** tab*

At measurement completion, the concentrations of the measured sample as well as the modules are computed and stored in the measure.mdb database. These results can be printed by means of the QUERYRES program by using a given formatting. QUERYRES makes it possible to include the modules in the printout. For that, do as follows:

1. While editing the formatting by means of the QUERYRES program (launched by clicking on the **Results Manager** icon), click on the **Modules/Input/Database** tab.
2. Click on the **Import** button located upon the **Modules** list, select the MLB file containing the modules that you want to insert, and then click on **Open**.
3. If you want to rename this module, enter the new name in the **New name** text box.
4. If you want to change the format of selected module, click on the button located underneath the **New name** text box. Notice that if you use a format based on a real or integer, QUERYRES lets you customize the unit name and the number of decimals.
5. Click on the **Add to Output** button to insert the selected column into the list of columns. Notice that the corresponding field disappears from the **Modules** list.

To clear this list, click on the **Clear** button.

Note: Modules are computed only if following conditions are both fulfilled:

- The name of the MLB file is the same as the measurement method name.
- The MLB file is located in a specific directory that is by default the `C:\Spectra EDX\Libraries\MeasMethods\` directory.