

Figure 143 Percentage file, scans for the percentages

Back in the Scan tree add another scan for the percentage value to be read into.

Select the **MID** tab and then input the following:

Available to Scan: none

Scan Legend: N2 %

as shown in Figure 143.

In the **Faraday** box change the available input to f(%).

Repeat the above for O₂ and Ar scans

Refer to Figure 143.

Finally, in the scan tree double click on the **Events** box.

In the Events editor right click on **Events** and select **f(x)input device**.

Double click on **f(x)1** to open the **f(x)input device editor**.

In the **f(x)input device editor** dialog box input the following:

Scan	Scan 4: N2 % 0.4
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Run Event Sequence	EventSequence1
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Get input value from	28_per
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Click **OK**

Create two more f(x) input devices for O₂ and Ar

Refer to Figure 144.

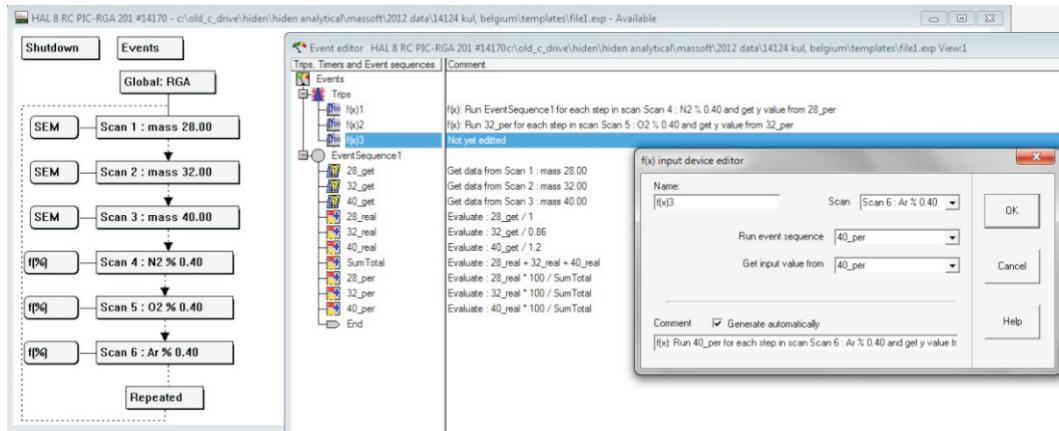


Figure 144 Percentage file, f(x) input device editor

Now when you start the scan you can view the raw pressure data of each gas as well as the percentage values displayed in real time.

5.2.3 A PPM file

A PPM file is created using the same steps as a percentage file with the exception of multiplying by 1000000 instead of 100 in the event sequence. Refer to Figure 145.

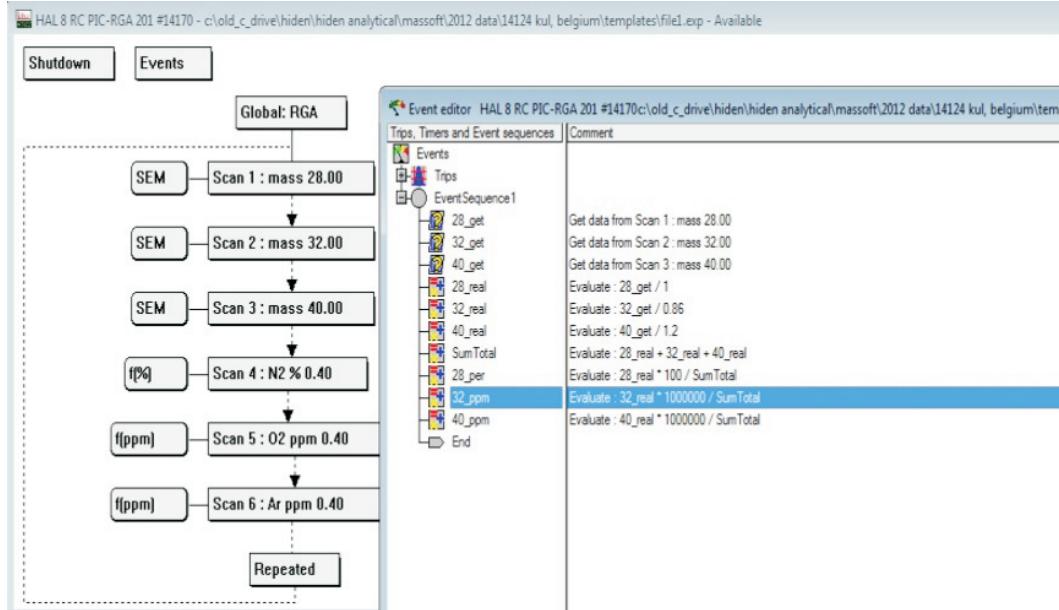


Figure 145 PPM file

5.2.4 Removing cracking pattern overlaps

A event sequence can be used to remove cracking pattern overlaps as the following example shows.

Let us suppose there is a gas mixture comprising 75% nitrogen and 25% carbon dioxide.

The cracking patterns for both gases are shown below.

	12	13	14	16	22	28	29	44	45	46
N ₂			7.2			100	0.8			
CO ₂	6	0.1		8.5	1.2	11.4	0.1	100	1.3	0.4

Both gases contribute to the mass 28 peak. Therefore, we cannot simply look at mass 28 for N₂ and mass 44 for CO₂ as approximately 11.4% of the mass 28 peak is due to CO₂.

Knowing this relationship however means that we can calculate the contribution from CO₂ at mass 28 and remove it, leaving just N₂ at mass 28.

This can be done using the following event sequence.

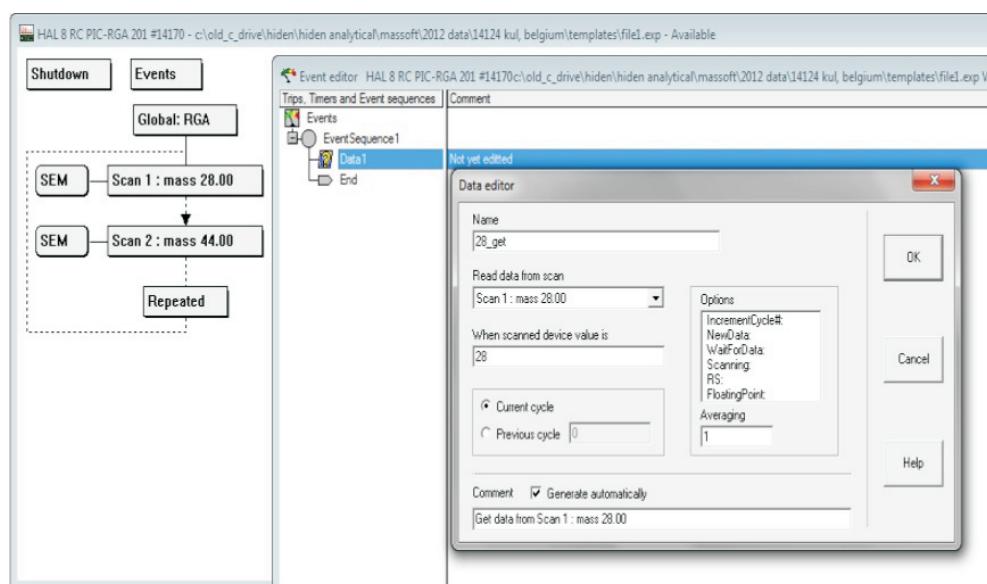


Figure 146 Overlaps, Data editor

Firstly two MID scans are made to monitor mass 28 and mass 44.

In the scan tree double click on **Events** to open the **Event editor**.

In the Event editor right click on **Events** and select **Data event**.

Double click on **Data1** to open the **Data editor** dialog box, as shown in Figure 146.

In the **Data editor** dialog box input the following:

Name	28_get
Read data from scan	Scan1: mass 28
When scanned device value is	28

Click **OK**

Create another Data event line for mass 44.

Right click on **44_get** and select **Evaluate event**.

Double click on **Eval1** in the **Evaluate expression editor** dialog box input the following:

Name	CO2at28
Equals=	44_get
/	100
x	11.4

Refer to Figure 147.

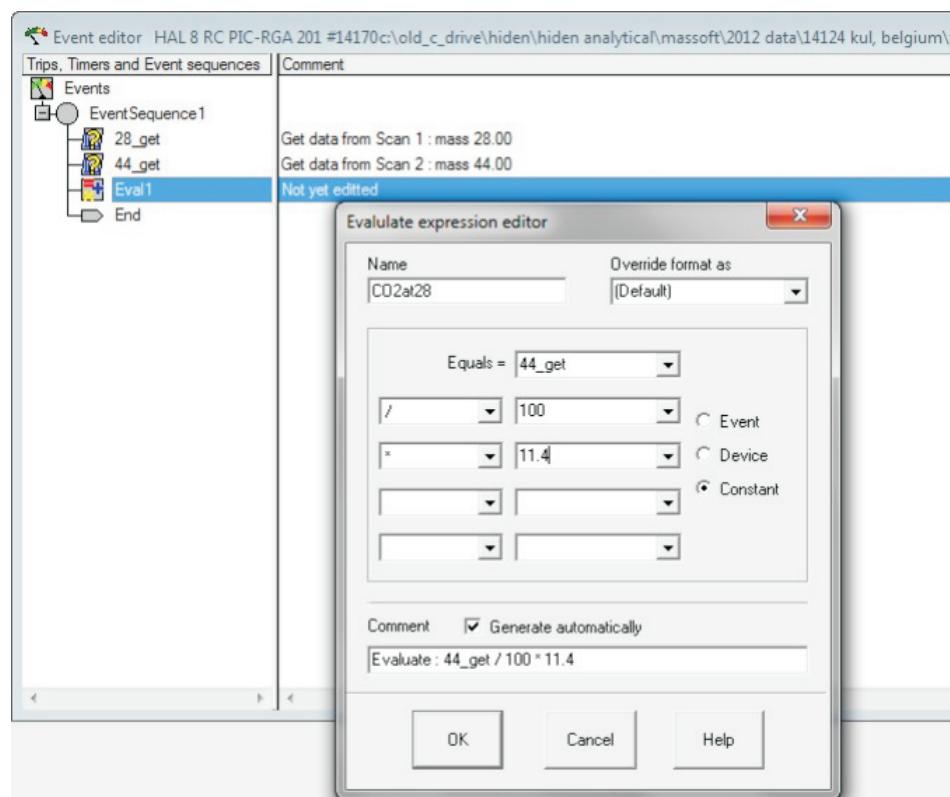


Figure 147 Overlaps, Evaluate expression editor

Click **OK**

This is the contribution of CO₂ at mass 28

Create another Evaluate event line.

In the **Evaluate expression editor** dialog box input the following:

Name	N2
Equals=	28_get
-	CO2at28

This is the intensity at mass 28 with the calculated contribution from CO₂ removed.

Back in the Scan tree add another scan box for the N₂ value to be read into.

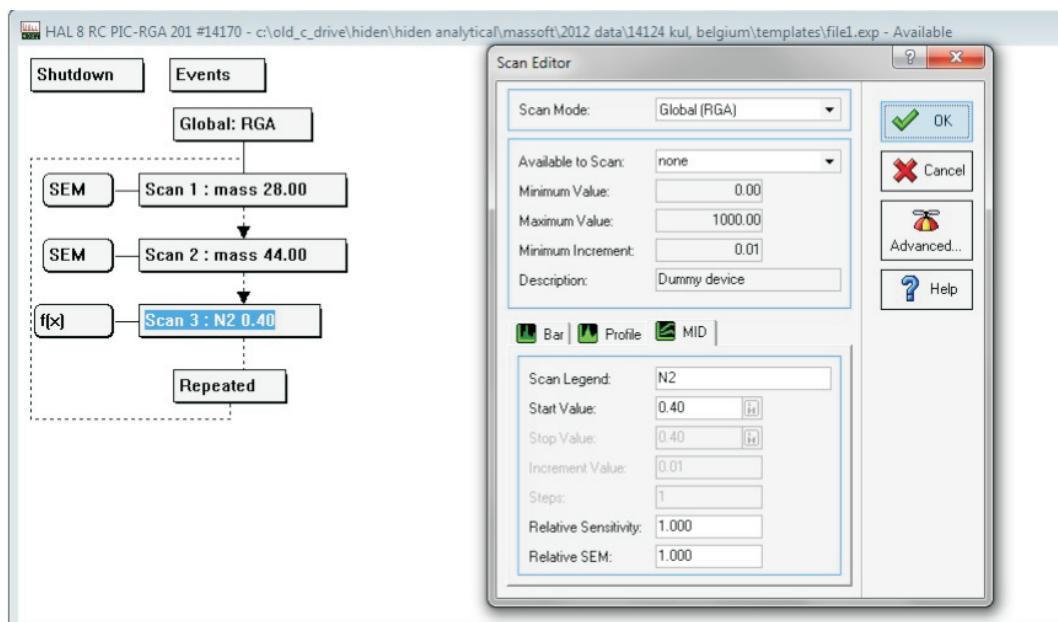


Figure 148 Overlaps, Scan 3

Select MID scan and enter:

Available to Scan: none

Scan Legend: N2

In the **Faraday** box change the available input to **f(x)** or **f(torr)**.

Finally, in the scan tree double click on the **Events** box to open the **Event editor**.

In the **Event editor** right click on **Events** and select **f(x)input device**

Double click on **f(x)1** to open the **f(x)input device editor**.

In the **f(x)input device editor** dialog box input the following:

Scan	Scan 3: N2 0.4
Run Event Sequence	EventSequence1
Get input value from	N2

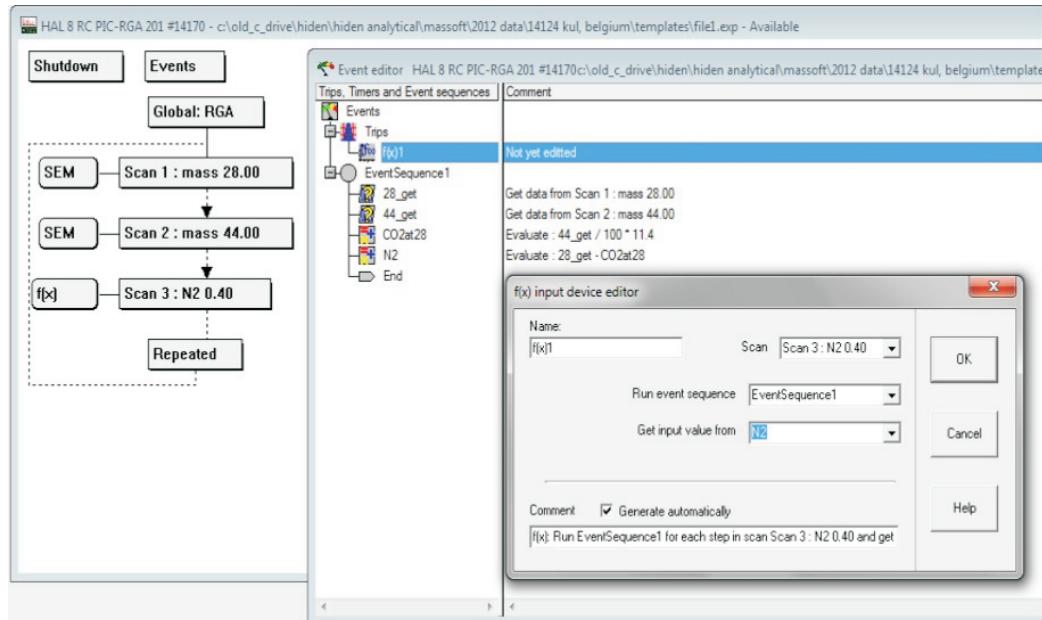


Figure 149 Overlaps, Scan 3

Now when you start the scan, scan 3 will show the N_2 intensity and scan 2 will show the CO_2 intensity.

Scan 1 shows N_2 with some contribution from CO_2 .

5.3 Calibration

5.3.1 Assumptions

There are two assumptions made when creating a percentage or ppm file.

1. Where overlaps are present you are assuming the ratio between calculated peak intensities is correct.

The ratio between peaks in cracking patterns can vary slightly from one mass spectrometer to another. The library values are used as a guide.

For complete accuracy, where overlaps are present and spectral peak relationships are being relied upon the ratio between peaks should be calculated by sampling the pure gas.

Once this has been done once for this gas you will not have to do it again. Just use this value in the cracking pattern instead of the library value. The Hiden library can be edited accordingly.

2. Library RS factors have been used.

Once you have created your percentage or ppm file you need to compare it against a known gas mix in order to calibrate the file. The mass spectrometer should be connected to a calibrated gas bottle/MFC set-up that gives a known gas mix at the approximate levels of the gases you are interested in.

The mass spectrometer should be allowed to sample from this gas mix and run for several minutes (30 minutes ideally) to make sure that the sample line is fully flushed and signals are stable.

When the percentage or ppm file is run the percentage values may not be the same as the values we know the mass spectrometer is sampling.

To calibrate the file the RS values should be edited in the event sequence to correct the reading.

The file should be stopped, edited and then started again.

The RS factors can be calculated manually using the formulas below:

Set the Bulk gas RS value to 1.

Then for the remaining gases:

$$RS = \frac{\text{Raw Torr}}{\% \text{ Correct}} \times \frac{\text{Bulk \% Correct}}{\text{Raw Bulk}}$$

or

$$RS = \text{Raw Torr} \times \frac{100}{\% \text{ Correct} \times \text{Sum Total}}$$

For a bulk gas with ppm mix:

The bulk gas RS is set to 1.

Then for each gas:

$$\left[\frac{\text{Raw Torr of gas}}{\text{Raw Torr of bulk}} \times 1000000 \right] \div \text{Gas ppm value in calibration bottle}$$

Or a file can be created to calculate the RS factors for you.

5.3.2 File to Calculate RS factors

This file will calculate the correct RS values using the first formula from Section 5.3.1 in order to calibrate a file ready for a gas mix.

This example will be for a calibrated air mix: 78% N₂, 21% O₂, 1% Ar.

As before, firstly create your file to monitor the desired masses, in this case MID scans of masses 28, 32 and 40.

In the scan tree double click on the **Events** box to open the **Event editor**.

Right click on **Events** and select **Evaluate event** from the list to add an Evaluate line.

Double click on **Eval1** to open the **Evaluate expression editor**.

In the **Evaluate expression editor** dialog box input the following:

Name	N2_%_in_mix
Equals=	78

This is where you enter the known percentage gas level in your calibrated gas mix.

For N₂ this is 78 as air is 78% N₂.

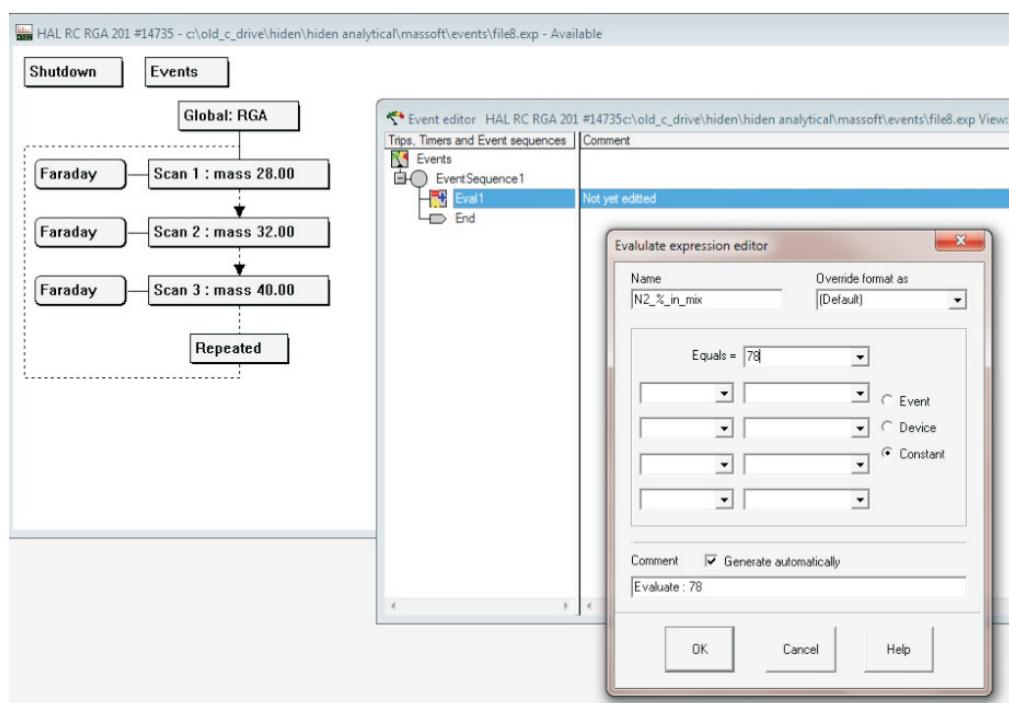


Figure 150 Calculate RS factors

Repeat the above for the remainder of the gases in your mix.

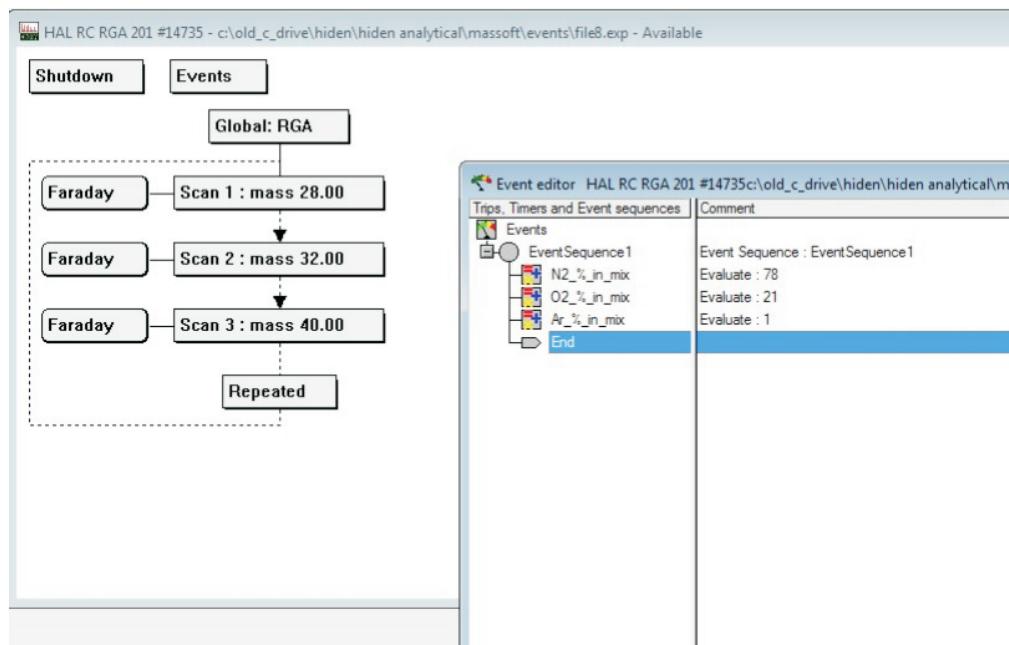


Figure 151 Calculate RS factors, gas mix

As before, link the data from a scan into the Event editor box by adding a Data event line to the event sequence. See Figure 152.

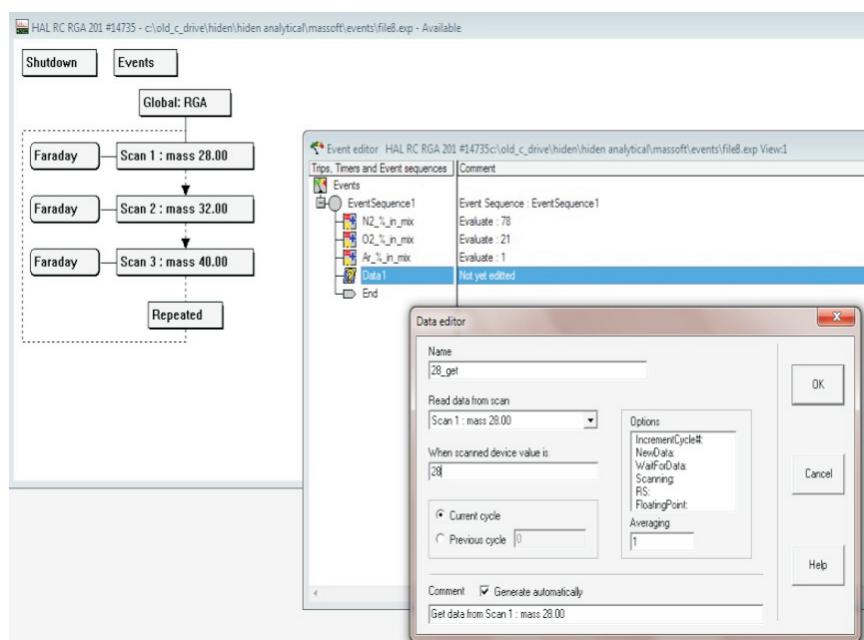


Figure 152 Calculate RS factors, Data editor

Repeat for the remaining gases.

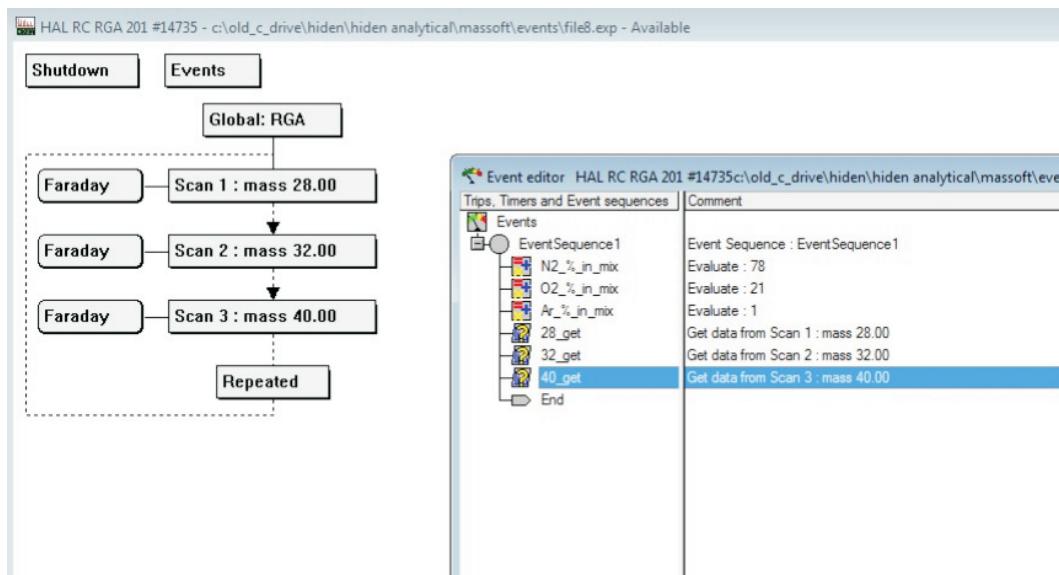


Figure 153 Get data from three scans

Now we need to calculate the correct RS factors required for our known calibrated gas mix. Remember the bulk gas RS value will be 1. In this example N2 is the bulk gas.

This is done using the following calculation:

$$x_{RS} = \frac{x_{get}}{x\% \text{ in mix}} \times \frac{\text{N2 \% in Mix}}{\text{N2}_\text{get}}$$

Add a new Evaluate line to calculate the above equation for each gas, as shown in Figure 154.

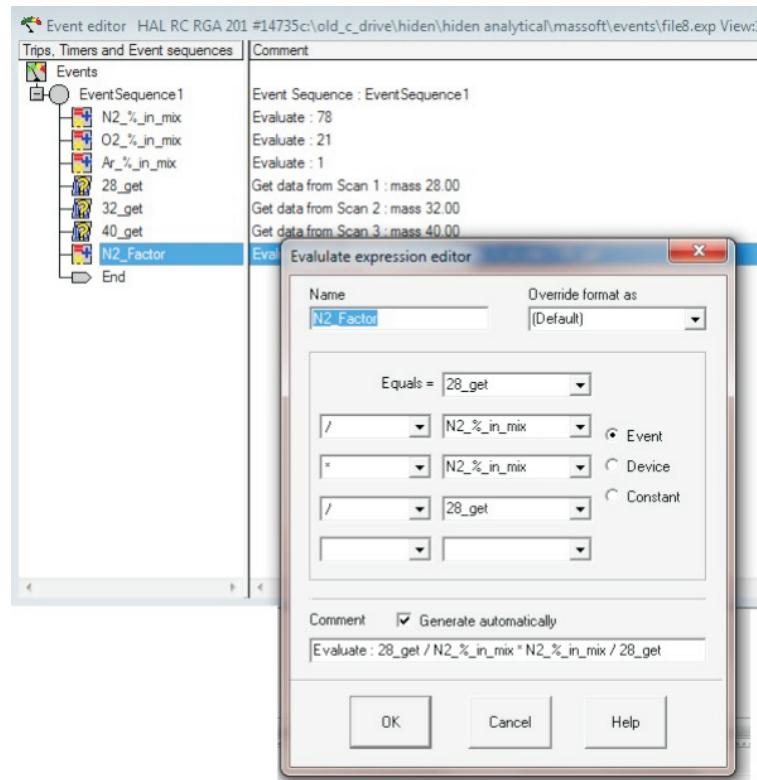


Figure 154 Evaluate N2 factor

Add Evaluate line to calculate the factors for O₂ and Ar.

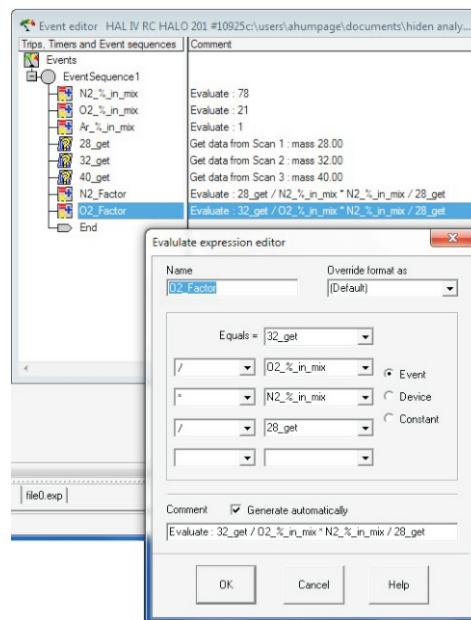


Figure 155 Evaluate O2

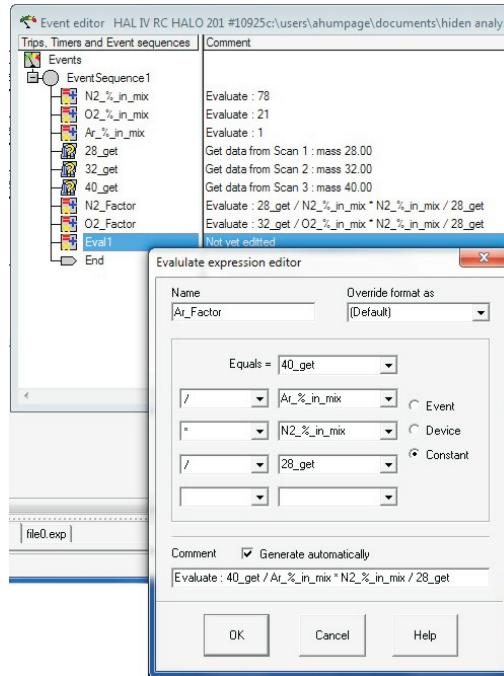


Figure 156 Evaluate Ar

Finally link the calculated factors back into the scan tree so we can see the results on the screen in real time.

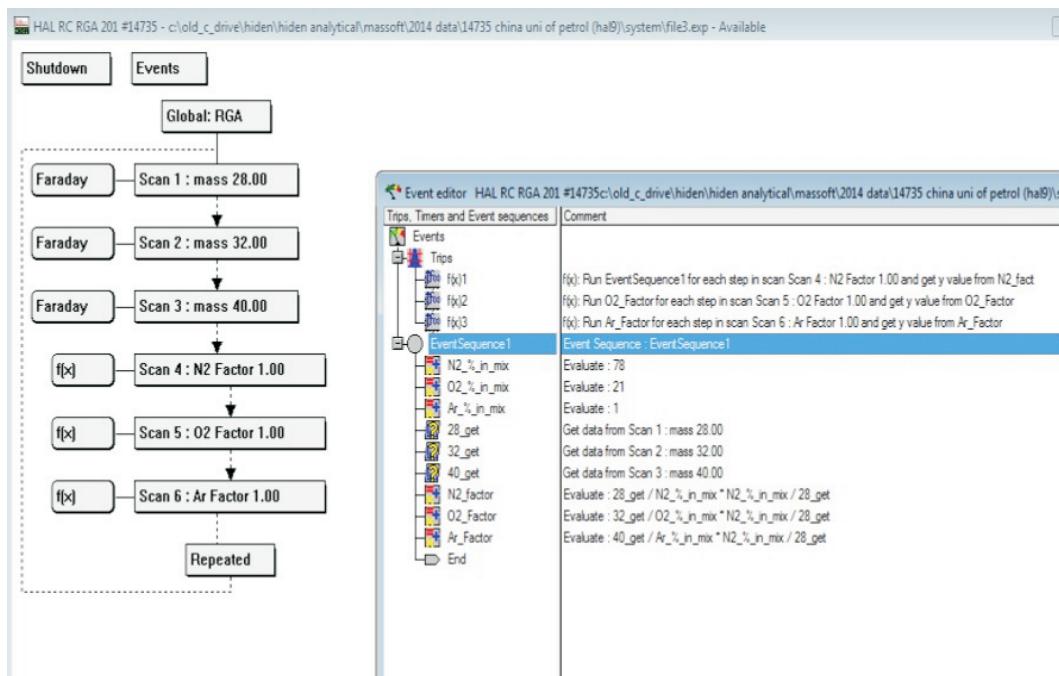


Figure 157 Link factors into scan tree

So now when you want to calculate the RS factors to calibrate a file:

- a) Connect your known calibration gas mix
- b) Allow 30 minutes of sampling with the mass spectrometer running to ensure the gas lines are fully flushed and readings are stable
- c) Enter the percentage levels of the calibration gas mix for each gas in the first few lines of the RS factor event sequence (N2_%_in_mix etc)
- d) Run the File
- e) Enter the new RS factors into your percentage file

Your percentage file is now calibrated against a known gas mix and ready to run.

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