

Quantitative Method Development

Monitor Instruments' Gas-Wizard™ software guides Series 3000 Cycloidal Mass Spectrometer users through the entire gas analysis method development, from start to finish. No prior experience in mass spectrometry or gas analysis is required.

To establish a quantitative method in Gas-Wizard, a file is created using the screen shown in Figure 1. This names the application and defines the number of process streams to be analyzed, the number of standards, and the calibration methods to be used in the application.

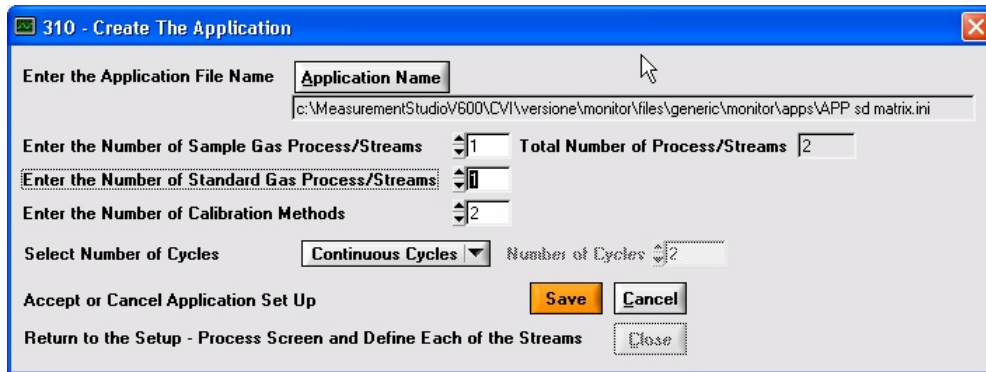


Figure 1. Application File Creation Screen

The next step is to define the indicator masses for the chemical components in each sample stream. The convenient on-line compound editor shown in Figure 2 simplifies this process.

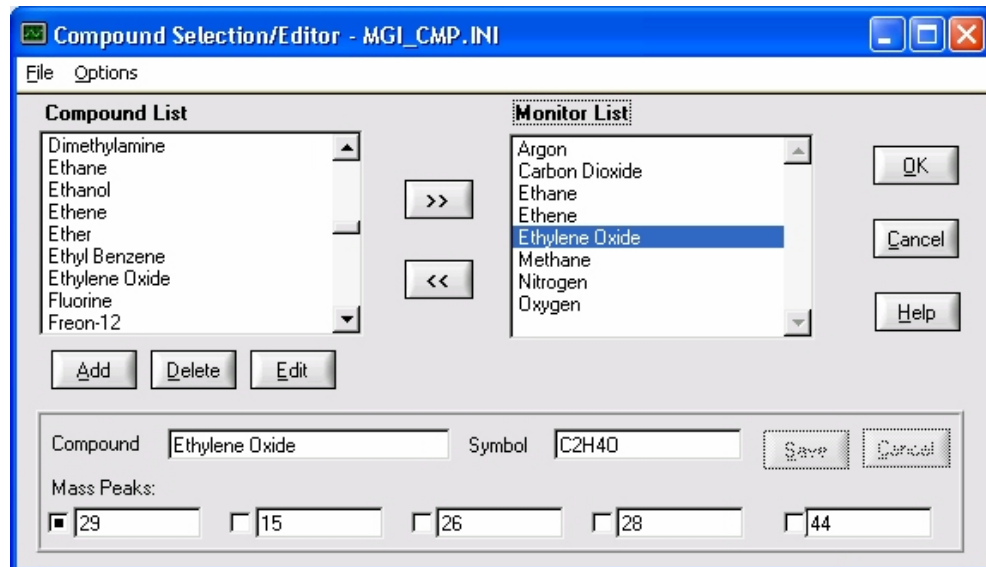
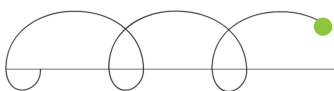


Figure 2. Compound Editor Screen

In this way, a process specification like that shown in the upper portion of Figure 3 is completed for each stream. The lower portion of this screen is used to structure the order, duration and frequency that each



stream is measured. Note that critical streams can be measured repetitively or more frequently in the sequence, according to the unique requirements of the application.

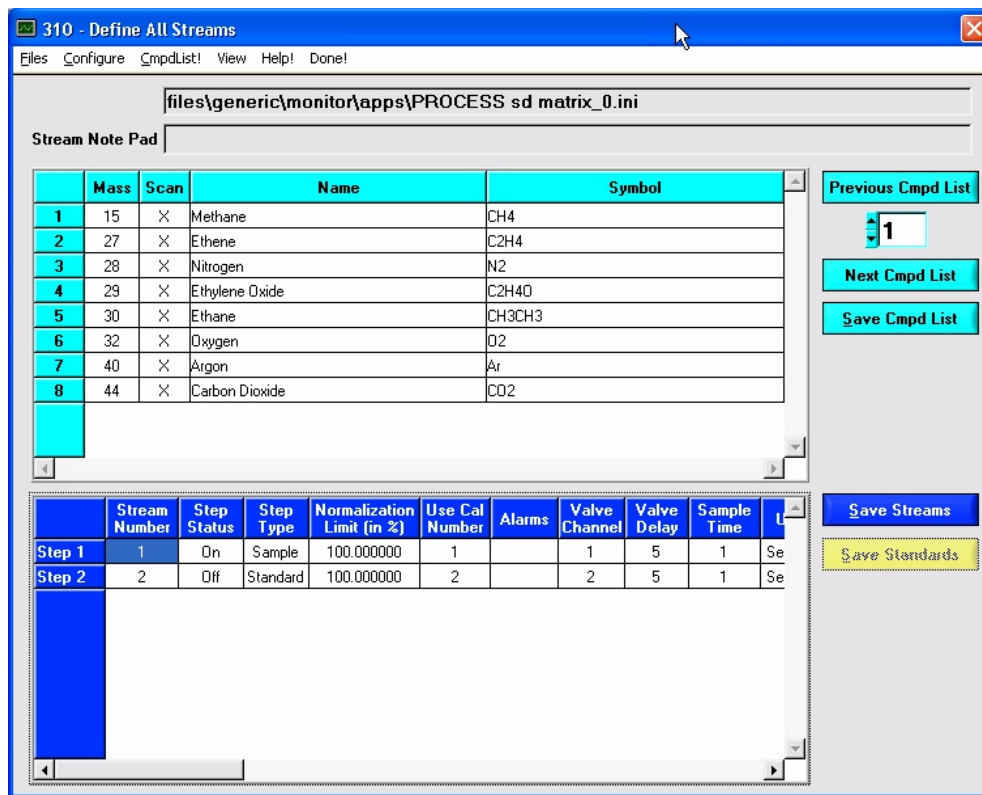


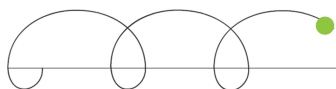
Figure 3: The Process Stream Specification screen is used to select indicator masses for each compound, and to schedule the sequence of process stream measurements. This example shows a typical component list for an ethylene oxide process stream.

A Calibration Screen, like that in Figure 4, is constructed for each calibration method. It has three sections. At the top, a fragmentation matrix table summarizes the indicator masses to be measured (columns) and the stream components (rows). The indicator mass for each gas is shown in red, while any spectral interferences are shown in yellow. The interferences will be resolved by the internal matrix inversion algorithm. Calibration gases containing the interfering compounds are used to establish the parameters for this calculation.

The middle section of the Calibration Screen is used to define the concentrations of gas standards used to measure detection response and thereby determine sensitivity. The bottom section of the screen displays the Calibration Methods Table that lists those methods which will be used in the application.

There are six types of calibration methods defined in the system software; each can be used on a stream specific basis depending on the application. These are as follows:

- Peak height
- Matrix deconvoluted peak height
- Normalization of raw intensities
- Matrix deconvoluted normalized raw intensities
- External Standardization
- External standardization with matrix deconvolution



The number of fragmentation calibration gases and sensitivity calibration mixtures used for a calibration method is input in the calibration methods table. Gas-Wizard will allow up to 256 calibration methods, each consisting of up to 30 sensitivity and 30 fragment pattern standards.

Table 3 - Fragmentation Matrix Table

	15	27	28	29	30	32	40	44	Frag Cal Order	Cal Valve Channel
CH4	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0	1
C2H4	0.000000	1.000000	1.000000	1.000000	0.000000	0.000000	0.000000	0.000000	1	1
N2	0.000000	0.000000	1.000000	1.000000	0.000000	0.000000	0.000000	0.000000	2	1
C2H4O	1.000000	0.000000	1.000000	1.000000	0.000000	0.000000	0.000000	1.000000	3	1
CH3CH3	0.000000	1.000000	1.000000	1.000000	1.000000	0.000000	0.000000	0.000000	4	1
O2	0.000000	0.000000	0.000000	0.000000	0.000000	1.000000	0.000000	0.000000	5	1
Ar	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	1.000000	0.000000	0	1
CO2	0.000000	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	1.000000	5	1

Table 2 - Sensitivity Measurements Table

	CH4	C2H4	N2	C2H4O	CH3CH3	O2	Ar	CO2	Deconvolute
Sensitivity #1	56%	18%	3%	.5%	11.5%		1%	10%	Yes
Sensitivity #2						20.95%			No

Table 1 - Calibration Methods Table

	Calibration Type	Frag Number	Sensitivity Number	Delta %	Number of Injections
Method # 1	Matrix/Normalize	5	2	0.10	1
Method # 2	Direct Ratio	0	1	0.10	1

Figure 4: The Calibration Screen allows the user to visualize the masses monitored for each component gas and any spectral interferences. Gas standards and calibration methods are defined in the lower parts of this screen. The ethylene oxide analysis shown has one calibration method consisting of 2 sensitivity calibrations and 5 fragmentation calibrations.

Gas-Wizard™ is both extremely flexible and easy to use. An explicit manual and helpful prompts for input screens minimize training requirements. In addition, method integrity is assured by a three level password protected hierarchy. Analytical method access can therefore be limited to designated personnel. At the same time, running established methods is simplified to a “one button” screen entry for plant operators.

Monitor Instruments’ Series 3000 cycloidal mass spectrometers provide process analysis in a wide variety of industries. Our application specific inlet systems, versatile Gas-Wizard™ software, and stable analyzers assure cost effective, high quality process control information. We invite you to visit our website (www.monitorinstruments.com), to request information via e-mail at info@monitorinstruments.com, or post at 290 East Union Rd., Cheswick, PA 15024, USA, or to contact us by telephone at +1.724.265.1212 or fax at +1.274.265.1199. We will give your application the careful, confidential consideration it deserves.

