

Catalyst Gas Monitoring and Control.

Aspec. Application Note

Speed and flexibility:

The Aspec Quadrupole Mass Spectrometer system is an ideal analysis tool for real time measurements and monitoring.

By connecting the specially designed, heated Aspec QMS sample Inlet probe, evolved gases from a process within a reactor can be measured and recorded with respect to time.

This example of a typical Catalyst driven Polyethylene reaction helps to demonstrate the capability of the Aspec QMS instrument.

Typical Polyethylene reactor using the Aspec QMS.



Typical Catalyst Process monitoring and control.

The Aspec QMS instrument is ideal for this type of application. It easily connects to the vent to enable the measurement of continuously, evolved gases from entire reaction. With a typical overall response time of less than 80ms, "Real Time" reactive profiling can therefore take place.

In this example:

The Aspec QMS instrument may be linked to a typical Polyethylene Catalyst reactor system to provide 2 types of analysis and control:

- 1) Direct feedback monitoring and control of Gas Phase Composition.
- 2) Calibrated, continuous record of entire gas phase

Control of Gas Phase Composition.

The Aspec QMS instrument may be connected to a Polyethylene reactor by means of a fast capillary sample line connected to the reactor Vent port.

A small sample gas bleed of around 50ml/min from the reactor is set and bled to atmospheric pressure. This is how gas is sampled (no sample conditioning necessary).

The Aspec QMS is set in software to continuously measure Hexane, Ethylene and Hydrogen in real time.

As the Aspec QMS is capable of updating each gas signal at rates of up to 10ms/gas an accurate profile of each gas profile is recorded and concentrations of each gas are collected and compared with respect to each other and with respect to the time within the process.

Using the in built Dynamic Data Exchange (DDE) function data may be "poked" in real time into other windows programs such as Excel for online data processing and monitoring.

Control of Gas Phase Composition.



The data above shows a typical profiles of initial changes of each of the gas components followed by closed loop control of each component via MFC,s to control the gas phase composition..

Calibrated Real time Monitoring of Reactor gas Composition.



The data above shows a typical real-time profiles of the entire reaction. Up to 64 different gas special my be set in the software and data collected and plotted at speeds of up to 60ms cycles (6 gases at 10ms/gas in this example) so precise profiling is possible.

This gives the user advantages over other analysis techniques such as GC and allows for maximum efficiency of the reactive process.

Data analysis



Temperature, weight loss and mass spectra data axis may be re-labelled and collected data automatically re-plotted into other formats

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Software control over peripheral instrument signal inputs (temperature and weight loss) allows interfacing/scaling of signals.

Mass Spectrometer data Analysis modes

The Mass Spectrometer instrument is an extremely fast and flexible instrument and has the capability to measure up to 64 gas species at any one time.

- The choice of gas species may be selected by the operator at any time or a standard matrix of gas species may be stored under a single analysis file and launched when required.
- Here are 3 analysis mode examples that demonstrate the capability and power of the Mass Spectrometer instrument
- Raw data **scan** mode.
- **Background** process **subtraction** (for looking at unknowns)
- Full **Calibration data** collection mode and data logging WRT time

Raw Gas/Mass scan Mode



In this mode, you can "scan" the entire mass range of the instrument in less than 2 seconds and produce a complete spectra of any gas composition. The spectra will automatically show very low as well as very high concentrations all on one single spectra. Each bar of the graph above represents a different gas or isotope of a gas. The higher the signal, the more gas there is.

This mode enables the user to quickly see if the gas composition is accurate and correct.

Background subtraction



This mode enables the operator to monitor a process for any changes that may occur. Any difference in gas composition can easily be logged and displayed on the bottom "Difference" axis. The acquired spectra may be interrogated and compared with a spectra library for identification of new, evolved gas species at any time.

Gas Identification



Continuously stored data may be interrogated at any time and correlated with known spectra either from the built in spectra library data base or from a remote spectra source such as NIST.

Full calibration Data Mode



This mode the is the most commonly used mode. It enables the user to calibrate and display up to 64 gas species and measure in direct concentration. Each gas component is calibrated by a set up routine and once calibrated the instrument will measure, data log and display the data in real time.

The above example shows a simple calibration and data logging of 4 common components that appear in air. All axis can be modified depending on the process and reaction you are wanting to measure.