

Note #06/07

Catalysis, Combustion and Fuel Cell Applications: Improving Data Quality When Nitrogen and Carbon Monoxide Levels Vary

BACKGROUND

Using mass spectrometry to measure the composition of gas mixtures is a well established technique in research for catalysis and fuel cell applications. The ability to measure multiple gas species in real time, with a fast response to changes in the gas composition, make it an ideal tool for characterizing a particular system under varying conditions. The benefits of the MKS Spectra™ Cirrus™ are explained in more detail in application note #01/05 (Overview of the Cirrus Gas Monitor in General Catalysis and Fuel Cell Applications). However, for some applications the use of mass spectrometry can be problematic due to interferences in the simultaneous measurement of carbon monoxide and nitrogen.

The molecular weight of both N₂ and CO is 28 and so the major peaks of both species appear at the same overlapping point in the mass spectrum of a quadrupole based mass spectrometer. For the applications of gas combustion, petrochemical catalysis and fuel cells this presents a problem as the level of CO is one of the measured parameters used to calculate reaction efficiency.

It is possible, in many applications, to use mathematical corrections to interpolate the levels of N₂ and CO from a mass spectrum. However, many of these rely on other parameters remaining stable, which is not always the case. Examples of where corrections can be used are given below:

- If air is used as the oxidant feed to a reaction and there is no other source of N₂, the constant level of argon in air (0.934% by volume) can be used to correct for the N₂ presence (78.084% by volume).
 - Due to the high level of nitrogen in air, any imprecision in the measurement leads to large errors in the CO measurement after subtracting the N₂ signal contribution at mass 28.
- The level of N₂ can be inferred from the measurement of N at mass 14 using a correction for the fraction of N₂ in the ionization source that would break down into N⁺ seen in the mass spectrum.
 - This relies on the N₂/N ratio remaining constant under all the measurement conditions and that there are no interferences at mass 14 from the fragmentation of any organic molecules in the ion source (CH₂⁺ also has a peak at mass 14).

- The level of CO could be inferred from the level of C at mass 12 (similar to the nitrogen correction), but this also relies on a constant CO/C ratio and no interferences from other carbon sources which is highly unlikely in fuel cells and catalysis.

SOLUTION

If a dedicated carbon monoxide sensor was used in parallel to the Cirrus mass spectrometer, the interference of nitrogen on the CO measurement would be removed. Such detectors are available, but the final analytical system would still have to meet the following criteria:

- The CO sensor would need to be tolerant to the presence of all the gas species typically found in fuel cell, catalysis and combustion study environments.
 - Tin oxide electrochemical detectors are inexpensive but they are common feed gas for fuel cell systems and catalysis experiments.
- The CO sensor would need to be as responsive as the mass spectrometer in order to provide meaningful data that correlated with the signals from the Cirrus.
- The CO sensor data would need to be captured within the Cirrus software and converted to meaningful concentrations that can be used to correct measured values of nitrogen where necessary.
- The CO sensor would need to be controlled from the Cirrus software to allow a completely integrated failsafe system for commercial use.

The nondispersive infrared (NDIR) CO sensor available as an option for the Cirrus fulfills all of this criteria, resulting in a gas analysis system designed specifically for fuel cell, catalysis and combustion studies. The integration of the sensor into the Cirrus Process Eye™ Professional software is shown in Figure 1.

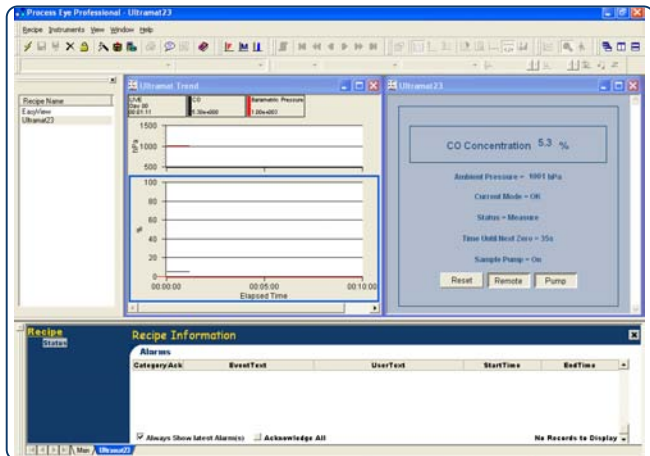


Figure 1. Integration of the NDIR sensor with Process Eye™ Professional software



Figure 2. NDIR sensor and Cirrus™ combined to form one complete system

The CO sensor is available with different configurations to suit particular needs for analytical precision and concentration ranges. Each sensor is simply integrated into the Cirrus software to enable transparent reporting of gas composition for a wide variety of conditions. The CO sensor can also be physically integrated with the Cirrus system in different ways to accommodate the needs of the user. Figure 2 shows the CO sensor fitted into a 19-inch rack mount mobile cabinet with the Cirrus, so the complete system can be moved between sampling sites within a facility.

CONCLUSION

The problem of data accuracy for carbon monoxide determination in the presence of nitrogen, organic carbon and hydrogen for catalysis studies, has been overcome by the use of an NDIR sensor integrated with the Cirrus mass spectrometer. The total system is turn-key and offers all the benefits of a mass spectrometer with interference free measurement of CO. Key benefits of the system include:

- Simultaneous multiple gas species analysis
- Determination of all gas species
- Real time signals
- Fast response to gas composition changes
- Wide dynamic range of measurement

For further information, call your local MKS Sales Engineer or contact the MKS Applications Engineering Group at 800-227-8766. Spectra™, Process Eye™, and Cirrus™ are trademarks of MKS Instruments, Inc., Andover, MA.