



Limit of Detection study using Aspectrics MultiComponent™ Analyzers and integrated sampling cell.

SUMMARY: *when dealing with the quantitative analysis of IR-absorbing chemicals in gas phase, an ever-present question is that of the limit of detection of the method. This technical note reports the experimental results obtained when testing this parameter using various configurations of Aspectrics EP-IR based MultiComponent™ Analyzers and using dedicated gas cell sampling accessories of various pathlength for integrations times ranging from 5 to 60 seconds. This report is not meant to be all-inclusive, but simply a representation of the analytical capabilities of EP-IR spectrometers.*

INTRODUCTION

Encoded Photometric InfraRed (EP-IR) spectroscopy is a novel way to capture the entirety of the IR signal generated by IR-absorbing chemicals. It relies upon the use of a spinning encoder disk to modulate up to 128 contiguous spectral regions (forming a complete spectrum) at various frequencies and recombining these modulated frequencies into an interferogram ready for mathematical analysis.

This technical note reports actual results for Limits of Detection (LODs) observed when using various configurations of EPIR spectrometers in relation with dedicated I-Cell multi-pass gas cell sampling accessories for integration times varying from 5 to 60 seconds.

MATERIALS & METHODS

- Instruments: EPIR MC5000A (128 channels; 2.50-5.00 μm nominal range) and MC5500A (128 channels; 2.85-5.50 μm nominal range)
- Gas Cells: I-Cell 2.0 meter and 3.2 meter pathlength multi-pass integrated gas cells with collimated 11W IR sources.
- Environmental: room temperature and pressure.
- Data Collect: 5.12 second or 1 minute integration (512 or 6000 scan boxcar average, respectively)
- Experimental: Data collected at concentrations of 0, 1% rel., 5% rel., 10% rel., 50% rel. and 100% relative of maximum concentration range.
2 independent sets of data were collected for each gas.

- Computations:
 - LOD Computations:
 - Method 1: LOD results computed according to VDI 4201 – VDI 4203 standards, i.e. computed as the Standard Error of Prediction (SEP) when applying an independent validation set of spectral data to calibration equation calculated for range of concentrations from 0-10% relative to maximum concentration of full calibration range.
 - Method 2: LOD results computed as the standard deviation of calculated values on a set of independent validation standards for a reference concentration value of "0."
 - All results reported as 1 sigma ($1*\sigma$). Reader should adjust results to $2.00*\sigma$, $2.54*\sigma$ or $\pm 3.00*\sigma$ depending on the level of certainty desired for the expression of LOD.

RESULTS & DISCUSSION

All results are reported in tables 1a and 1b, including:

- Chemical Information
 - Chemical name
 - Full range of concentrations
- Experimental LOD Results
 - Integration time
 - LOD (Method 1)
 - LOD (Method 2)
- Spectroscopic Conditions:
 - EPIR model
 - I-Cell pathlength



Table 1a: Experimental Results LODs with 5.12 sec. Integration Time

Chemical Information		Experimental Results		Spectroscopic Conditions	
Compound	Range	Integration Time	LOD Method 2	EPIR Spectrom.	Pathlength
Carbon Monoxide	0 - 2994 ppm	5.12 seconds	900 ppb	MC5500	2.0 meters
Nitrogen Dioxide	0 - 256 ppm	5.12 seconds	800 ppb	MC5500	2.0 meters
Methane	0 - 100 ppm	5.12 seconds	400 ppb	MC5500	2.0 meters
Nitric Oxide	0 - 296 ppm	5.12 seconds	4.1 ppm	MC5500	2.0 meters
Propane	0 - 641 ppm	5.12 seconds	400 ppb	MC5500	2.0 meters

Table 1b: Experimental Results LODs with 60.0 sec. Integration Time

Chemical Information		Experimental Results			Spectroscopic Conditions	
Compound	Range	Integration Time	LOD Method 1	LOD Method 2	EPIR Spectrom.	Pathlength
Acetylene	0 – 100 ppm	60.0 seconds	111 ppb	70 ppb	MC5000A	3.2 meters
Carbon Monoxide	0 – 50 ppm	60.0 seconds	225 ppb	173 ppb	MC5000A	3.2 meters
Ethane	0 – 100 ppm	60.0 seconds	70 ppb	34 ppb	MC5000A	3.2 meters
Ethylene	0 – 100 ppm	60.0 seconds	161 ppb	163 ppb	MC5000A	3.2 meters
Iso-pentane	0 – 10 ppm	60.0 seconds	17 ppb	8 ppb	MC5000A	3.2 meters
Methane	0 – 25 ppm	60.0 seconds	76 ppb	65 ppb	MC5000A	3.2 meters
Propylene	0 – 100 ppm	60.0 seconds	215 ppb	67 ppb	MC5000A	3.2 meters

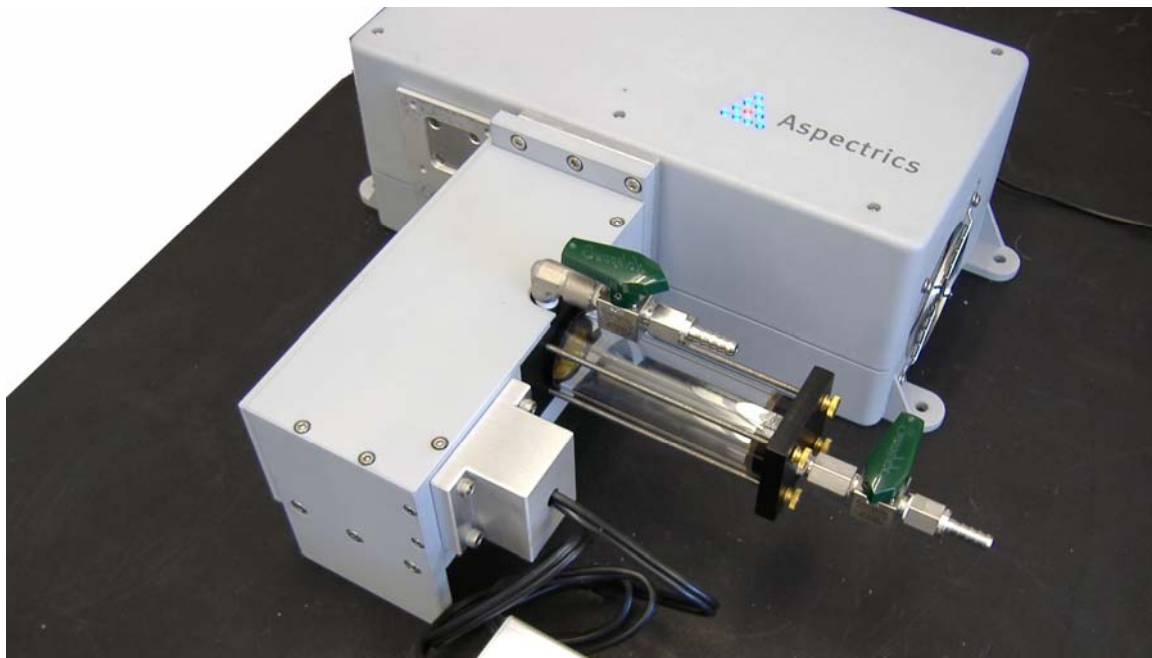


Figure 1:
Aspectrics
MultiComponent™
Analyzer with
integrated I-Cell™
dedicated gas
sampling accessory.

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