Detection and Quantitation of Carbonyl Sulfide, Using SIFT-MS

Carbonyl sulfide (COS; also known as carbon sulfoxide) was proposed as a fumigant[1] by the Stored Grain Research Laboratory of the Commonwealth Scientific and Industrial Research Organization (CSIRO) in Australia and was patented in 1992. The compound was seen as a possible replacement for methyl bromide and for use in situations where insect pests have developed a resistance to phosphine, but to date, its use has not become widespread.

Syft Technologies Voice200® Selected Ion Flow Tube Mass Spectrometry (SIFT-MS) instruments set the standard for simple and objective detection and quantitation of fumigants and volatile toxic industrial compounds (TICs) in shipping containers. In this report, we demonstrate the effectiveness of SIFT-MS in detecting carbonyl sulfide at relevant concentrations.

Experimental

Sample preparation

Carbonyl sulfide was synthesized by the reaction of ammonium thiocyanate and sulfuric acid. The crude gas was dried with calcium chloride and subsequently purified in several freeze/thaw cycles. The gas was analyzed using the Syft Technologies Voice200® SIFT-MS instrument to determine its purity (major contaminants were hydrogen sulfide and hydrogen cyanide at ~0.25% each). For a sample of known concentration the gas was diluted in dry nitrogen using standard gas-handling methods.

SIFT-MS

SIFT-MS is a powerful analytical technique that uses chemical ionization reactions coupled with mass spectrometric detection to rapidly quantify targeted VOCs. VOCs are identified and quantified in real time from whole-gas samples based on the known rate coefficients for reaction of the chemically ionizing species (so-called reagent ions) with the target analytes. The most common reagent ions used are H_3O^+, NO^+ and O_2^+, which react with trace VOCs in well characterized ways but *do not* react with the major components of air. Generally the soft chemical ionization used in SIFT-MS yields a smaller range of product ions than is common in electron impact mass spectrometry (as used by gas chromatography mass spectrometry (GC-MS), for example). Hence the need for gas chromatographic separation of the sample is circumvented, speeding sample throughput and providing instantaneous quantification of VOCs. Use of several reagent ions to independently quantify target analytes also greatly reduces interferences, markedly increasing the specificity of SIFT-MS versus competing whole-gas analysis technologies.

The Syft Technologies Voice200® SIFT-MS was run in two modes:

- Full Scan Mode (FSM): FSM aids identification of unknown compounds but also allows concentrations to be derived. In this case, full mass scans were obtained using each of the three standard SIFT-MS reagent ions (H_3O^+, NO^+ and O_2^+) over the mass range 15 to 200 Daltons to determine the purity of the COS sample.

- Selected Ion Mode (SIM): SIM targets specific compounds for sensitive quantitative analysis. All concentrations are shown in parts-per-billion by volume (ppb).

Results and Discussion

Full mass scan analysis of carbonyl sulfide diluted in nitrogen confirmed previous work[2] showing that there is no reaction with the H_3O^+ and NO^+ reagent ions and that a single product at m/z = 60 was observed with the O_2^+ reagent ion which corresponds to the production of the COS^+ ion.

The results obtained using a SIM method that targeted carbonyl sulfide are shown in Figure 1. A linear response was obtained for samples serially diluted samples in dry nitrogen. For five seconds sampling of the COS product ion, limits of quantitation (LOQ) and detection (LOD) of 3.1 ppb and 1.8 ppb, respectively, were obtained.[3] The primary cause of these elevated values is interference of the single available product mass with common compounds, such as acetic acid and the two propanol isomers. Although these values are somewhat above the natural atmospheric concentration of carbonyl sulfide (0.5 ± 0.05 ppb),[1] the human occupational exposure limit is rather high (100 ppm),[4] indicating that COS is not particularly toxic to humans. Hence the SIFT-MS technique provides an ideal solution for real-time monitoring of carbonyl sulfide on its own or as part of a larger fumigant suite.

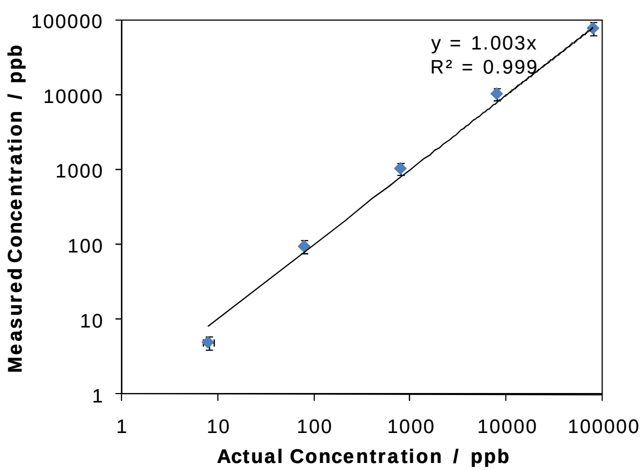

Figure 1. Linear detection of carbonyl sulfide using the Syft Voice200 SIFT-MS instrument.

Conclusion

The detection of carbonyl sulfide has been demonstrated using the Syft Voice200® SIFT-MS instrument. A linear response over at least four orders of magnitude was obtained, with a LOD of 1.8 ppb for a five-second measurement. These results show that SIFT-MS is well suited to the detection of carbonyl sulfide as it would be used in the fumigation industry.

For more information about this unique technology, please contact your nearest Syft Technologies office or visit www.syft.com.

References

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