Diacetyl Analysis, Using SIFT-MS

Diacetyl (2,3-butanedione) is one of the key flavor compounds in butter¹ and is used to imitate butter in preparations applied to microwave popcorn. Recently, diacetyl has been identified as a causative agent in the development of "popcorn worker's lung", a fixed obstructive lung disease – bronchiolitis obliterans – occurring in workers at factories producing microwave popcorn.² Understanding the avenues by which popcorn workers are exposed, and mitigating or eliminating them has become very important.

Detection of diacetyl using Selected Ion Flow Tube Mass Spectrometry (SIFT-MS) was first demonstrated in 1997.³ SIFT-MS provides realtime, quantitative analysis of volatile organic compounds (VOCs) in a range of environments to part-per-trillion-by-volume (ppt) levels, and is hence ideally suited to characterizing exposure to diacetyl.

In this report we demonstrate the linear response of a Syft Technologies Voice200[®] SIFT-MS instrument to diacetyl over the concentration range of 2 parts-per-billion by volume (ppb) to 20 parts-per-million by volume (ppm). We also demonstrate the ability of SIFT-MS to detect and quantify diacetyl in the presence of two potentially interfering isobaric compounds, hexane and 3-pentanone.

SIFT-MS

A new analytical technique, Selected Ion Flow Tube – Mass Spectrometry (SIFT-MS), identifies and quantifies Volatile Organic Chemicals (VOCs) directly from air in real-time. Based on sound principles of chemical ionization mass spectrometry and precisely controlled ion reaction kinetics, SIFT-MS uses a sequence of three reagent ions to resolve interfering species, differentiate isobaric compounds and produce intrinsically quantitative data without laborious calibration procedures. Three one-liter Tedlar gas sampling bags (SKC Inc.) were filled with one liter of high purity nitrogen gas. A 1-mL sample of vapor was taken from the headspace of commercial samples of diacetyl, hexane or 3-pentanone and injected into one of the bags. Each bag was then analyzed using the SIFT-MS instrument to ascertain the concentration of diacetyl, hexane or 3-pentanone, as appropriate.

From these, the serial dilutions of diacetyl were planned, and the amount of hexane or 3-pentanone to be spiked was determined. Serial dilutions of diacetyl were prepared in the range 2 ppb to 20 ppm and analyzed using the Voice200 instrument. Hexane was then spiked into each bag at a final concentration of ca. 0.5 ppm and instrumental analysis repeated. Finally, the bags were spiked to a 3-pentanone concentration of *ca*. 1.5 ppm and analyzed as before.

Figure 1 shows the response obtained for diacetyl over the concentration range from 2 ppb to 20 ppm. In Figure 2, the diacetyl concentrations are shown after approximately 0.5 ppm of hexane was added to each of the serial dilutions. The results obtained following addition of ca. 1.5 ppm of 3-pentanone to the dilutions are given in Figure 3.

The Syft Technologies Voice200[®] SIFT-MS instrument maintains a linear response to diacetyl from low-ppb to ppm levels in spite of the addition of the isobaric compounds, hexane and 3-pentanone.

Syft Technologies offers a gas sample collection system, shown in Figure 4, to facilitate analysis when the instrument is not located near a sampling point.



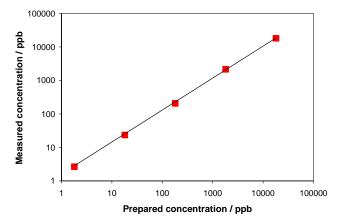


Figure 1. Concentrations of diacetyl determined using a Syft Technologies Voice200 SIFT-MS instrument after serial dilutions were made in Tedlar gas sampling bags filled with one liter of nitrogen.

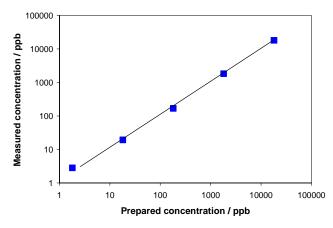


Figure 2. Concentrations of diacetyl in the samples shown in Figure 1 after approximately 0.5 ppm of hexane had been added to each bag.

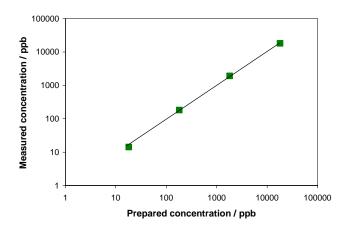


Figure 3. Concentrations of diacetyl in the samples shown in Figure 1 after approximately 0.5 ppm of hexane and 1.5 ppm of 3-pentanone had been added to each bag.



Figure 4. Syft Technologies' Sample Case holds three 1-liter Tedlar or Kynar sample bags, which are removed for Voice200 analysis as shown. The operator uses the integrated touch screen display to start testing and to view results.

THE VOICE200[®] SOLUTION. FAST, ACCURATE, SIMPLE.

Syft Technologies' Voice200 instrument can reliably quantify diacetyl to very low ppb concentrations in the presence of isobaric compounds. Specifically designed for ease of use, the push-button, stand-alone system requires minimal training for operation and provides instantaneous results.

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

References

- H.-D. Belitz, W. Grosch, P. Schieberle, P. (2004). Food Chemistry, 3rd Ed., Springer, Germany, p. 546-547.
- R. Kanwal, *et al.* (2006). "Evaluation of Flavorings-Related Lung Disease risk at Six Microwave Popcorn Plants." *J. Occup. Environ. Med.*, 48, 149-157. R. Boylstein, *et al.* (2006). "Diacetyl Emissions and Airborn Dust from Butter Flavorings Used in Microwave Popcorn Production." *J. Occup. Environ. Hyg.*, 3, 530-535.
- 3. P. Spanel, Y.F. Ji and D. Smith (1997). "SIFT studies of the reactions of H_3O^+ , NO^+ and O_2^+ with a series of aldehydes and ketones." *Int. J. Mass Spectrom. Ion Processes*, 165/166, 25-37.



International enquiries Syft Technologies Ltd. 3 Craft Place Middleton PO Box 28 149 Christchurch, New Zealand Website www.syft.com

Phone +64 3 338 6701 Facsimile +64 3 338 6704 Email sales@syft.com North American enquiries Syft Technologies Inc. 1525 Park Manor Blvd, Suite 272 Pittsburgh, PA15205 4805, USA Phone 888 200 5991 Email NAInfo@syft.com

RPT-004-01.0