SIFT-MS: A New Perspective on Monitoring of Occupational Chemical Exposure

Monitoring of worker exposure to toxic chemicals is receiving increasing attention from Occupational Safety and Health (OSH) regulators. Various methods – such as photoionization detectors (PIDs), chemical indicator tubes and gas chromatography (GC) – have traditionally been used to OSH monitoring and compliance. The results have been mixed.

Selected Ion Flow Tube Mass Spectrometry (SIFT-MS) is a proven technology used for real-time monitoring of air quality and non-invasive testing of human breath. Importantly, SIFT-MS provides analysis of raw whole-air samples – that is, analysis without sample preparation. SIFT-MS analysis of breath, in particular, offers significant opportunities for direct monitoring of air as it is inhaled by workers.

This whitepaper provides an overview of SIFT-MS and its suitability for OSH applications, particularly the monitoring of toxics on worker breath.

Introduction

Modern society relies on a range of industries that produce or use chemicals of varying toxicities, such as in the paint, printing and agrochemical industries. Protecting workers from unsafe exposure to these chemicals is increasingly capturing the attention of regulators, employers, and the workers themselves. This attention has highlighted the role of occupational safety and health (OSH) regulation, particularly with regard to identification and enforcement of minimum air quality standards for workplaces.

For situations where workers' exposure to hazardous substances cannot be practically eliminated, National OSH regulators publish standards listing maximum permissible exposure levels.

Table 1 lists some national and international organizations that set or recommend these standards, together with the terminology they use. These standards are produced based on available evidence linking chemical exposure to short- or long-term health effects.

In reality, occupational exposure standards are continually revised as the accumulation of toxicity data grows. For example, results of a study published in 2004 indicated benzene had detrimental effects on white blood cells at lower levels than were previously realized¹. White blood cell counts were found to decline in workers exposed to average benzene levels as low as 0.57 part per million (ppm), whereas the US Occupational Safety and Health Administration (OSHA) Permissible Exposure Limit (PEL) at the time was 1 ppm.

Methods for measuring occupational exposures

Many significant toxics (such as benzene, toluene, ethylbenzene the xylenes and formaldehyde) are volatile organic compounds (VOCs). Traditional methods for assessment of exposure to these include photoionization detectors (PIDs), chemical indicator tubes or off-site laboratory analysis of sampling bags or sorbent tubes by gas chromatography (GC). Table 2 presents a comparison of SIFT-MS with these traditional methods.

SIFT-MS instruments can be located on site, off site, or in a vehicle such as a van. When located on site or in a vehicle, SIFT-MS allows continuous live monitoring of air quality, with high sensitivity and specificity. When located off site, samples are collected via

Tedlar bags or sorbent tubes and transported to a laboratory-based instrument, which is usually in a commercial laboratory.

In all cases SIFT-MS allows rapid non-invasive analysis of air and breath samples, largely due to its ability to sample whole air without sample preparation or chromatographic separation.

The technical suitability of SIFT-MS for OSH applications

SIFT-MS allows rapid and continuous analysis of breath and whole air samples. It is a powerful analytical technique that uses chemical ionization

reactions coupled with mass spectrometric detection to rapidly quantify targeted VOCs^{2,3}. 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.

 $\rm H_3O^+$, $\rm NO^+$ and $\rm O_2^+$ reagent ions are used in SIFT-MS. These react with trace VOCs in well characterized ways but do not react with the major components of air. Generally the soft chemical ionization of SIFT-MS yields a much smaller range of product ions than is common in electron impact

mass spectrometry (as used by gas chromatography/mass spectrometry (GC/MS)). Hence the need for gas chromatographic separation of the sample is eliminated, speeding sample throughput and yielding instantaneous quantification of VOCs.

By using several reagent ions to independently quantify target analytes, SIFT-MS also greatly reduces interferences, markedly increasing the specificity versus competing whole-gas analysis technologies.

Standard SIFT-MS detection limits are in the low to sub- part-per-trillion (ppt) range.

Table 1. Some organizations that set or recommend occupational exposure limits

Organization	Country or region	Exposure Limit Name
National Occupational Health and Safety Commission (NOHSC)	Australia	National Exposure Standards
European Agency for Safety and Health at Work	European Community	Occupational Exposure Limits
Japanese Association of Industrial Health	Japan	Permissible Exposure Limits
Occupational Safety and Health Service	New Zealand	Workplace Exposure Standards
Health and Safety Executive (HSE)	UK	Occupational Exposure Standards
National Institute for Occupational Safety and Health (NIOSH)	USA	Recommended Exposure Limits
Occupational Safety and Health Administration (OSHA)	USA	Permissible Exposure Limits
American Conference of Governmental Industrial Hygienists (ACGIH)	USA	Threshold Limit Values

Table 2. A comparison of technologies used to monitor hazardous substances in the workplace.

Parameter	Photoionization Detectors (PIDs)	Chemical Indicator Tube	Gas Chromatography	SIFT-MS
Specificity	Very low	Moderate	High	High
Sensitivity	Moderate	Moderate	High	High
Analysis speed	Instant	Instant	Slow	Instant (on-site)¹
Consumable costs	Low	High	Moderate	Low
Cost per analysis	Low	High	High	Low to moderate
Subjectivity ²	High	High	Low	Low
Direct breath-sampling capability	No	No	No	Yes

^{1.} Rapid sample turnaround for off-site analysis using SIFT-MS.

^{2.} Subjectivity relates to human factors involved in interpretation of the analytical data provided.

Capabilities of SIFT-MS in OSH applications

A range of published reports describe the capabilities of SIFT-MS as a tool for non-invasive breath testing. Smith and Spanel⁴ and Smith et al.⁵ pioneered this area, including its validation. McEwan and co-workers have also published several papers in this area⁶⁻⁸, which validate SIFT-MS for use in breath analysis of several industrial VOCs.

As an example, Figure 1 shows SIFT-MS direct breath analysis of a volunteer exposed to fumes containing xylene and mesitylene7. Three breaths are shown. Measurements continued over the following four hours. Figure 2 presents only the mesitylene decay over this period, but it has a very similar form to xylene. It was observed that mesitylene was distributed within the body in two reservoirs with characteristic residence times, corresponding to different tissue types. For xylene, residence times of 0.4 and 2.5 hours were calculated. For mesitylene, residence times of 0.4 and 2.8 hours were calculated.

Figure 1. SIFT-MS Selected Ion Mode (SIM) measurements of xylene and mesitylene in the breath of a volunteer following a two-hour controlled exposure. The breath is sampled directly in real time and the concentration is expressed as parts per billion (ppb) by volume of the breath sample.

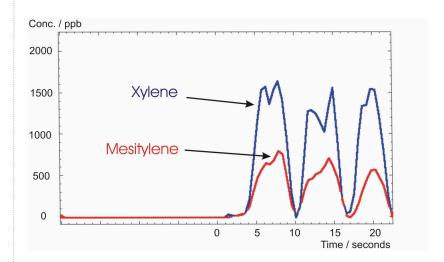
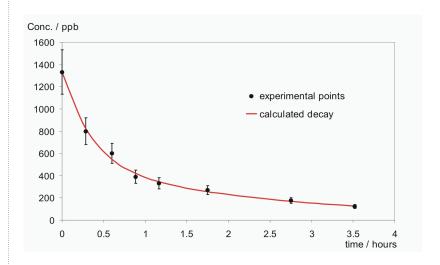


Figure 2. Decay of breath mesitylene level as measured by SIFT-MS from direct breath samples of a volunteer following a two-hour controlled exposure. The solid line represents a two-reservoir fit to the experimental points.



Practical limitations of common systems used to detect toxic volatiles in OSH applications

The ideal system for detecting toxic volatiles in OSH applications must accurately and clearly identify and quantify threats, while avoiding false positives and negatives.

A significant limitation of PIDs is that they indicate total levels of combined volatiles, rather than levels of individual volatiles. Alternatively, SIFT-MS identifies and quantifies individual volatiles, and multiple volatiles can be analyzed in a single scan.

Indicator tubes are subject to rather high levels of user subjectivity

and interpretation, and a tube of suitable concentration range must be pre-selected before analysis. Alternatively, SIFT-MS reports actual concentrations and can generate automated alert messages or alarms when concentrations exceed defined safe levels.

While GC/MS systems provide highly accurate and specific detection of volatiles, they are rather slow and require considerable expertise to operate and interpret results. Alternatively, SIFT-MS systems provide instantaneous results and can be configured for use by nontechnical personel.

References

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Conclusion

SIFT-MS provides the occupational safety and health sector with a powerful tool for quantitative and instantaneous measurement of hazardous volatile organic compounds in the workplace. With broad spectrum VOC analysis capabilities, it offers new opportunities in monitoring situations, allowing customization to a particular facility and the ability to adapt as needs change. SIFT-MS produces accurate analytical results that are readily compared to regulatory standards.

The high selectivity of SIFT-MS also enables simplified investigation of the synergistic effects of multiple VOCs.

The unique ability of SIFT-MS to sample breath and the headspace of blood and urine also means that there is now a rapid, effective and economical way to monitor VOC clearance rates.

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