SIFT-MS: A Significant New Tool for Real-Time Air Quality Monitoring

Volatile organic compounds (VOCs) are significant air pollutants. While air quality agencies and lawmakers recognize the public health issues associated with unmonitored and unquantified VOC pollution, until now there has been no entirely satisfactory way of routinely measuring a broad range of VOCs in real time and at the required sensitivities.

Selected Ion Flow Tube Mass Spectrometry (SIFT-MS) is the first technology that can quantify VOCs at the required levels and deliver benefits in ease of use, integration, remote operation and long-term calibration stability. SIFT-MS therefore presents a breakthrough in the detection, quantification and tracing of VOC hazards.

Introduction

Good air quality is an important contributor to quality of life, since pollution affects human health, property and the natural environment. Primarily formed by human activities, volatile organic compounds (VOCs) are significant pollutants that are often directly hazardous to human health and also contribute to secondary effects such as ozone production in photochemical-induced smog.

SIFT-MS is a unique technology that samples and analyzes whole air in real-time, to sub- part-per-trillion-by volume (pptv) level. SIFT-MS provides an ideal solution for monitoring VOCs and certain inorganic gases in ambient air.

This whitepaper briefly reviews the most important hazardous airborne volatile organic pollutants, then provides an overview of current air monitoring technologies, before presenting example data obtained from a SIFT-MS instrument used for detection of ambient VOCs.

Hazardous Airborne Volatile Organic Pollutants

VOCs are a diverse group of carbon-based compounds that exist either as gases or volatile liquids at room temperature. As well as causing direct negative health effects, VOCs are significant contributors to photochemical smog. Current methods to detect and quantify VOCs (and the associated health risks) often rely on the measurement of total non-methane organic compound (NMOC) concentration in the atmosphere or from a particular source. The NMOC concentration is then entered into accepted kinetic models for photochemical smog formation.

Unfortunately, measuring total concentrations of VOCs in air samples does not provide a reliable indication of potential health effects from air pollution. This is because VOCs differ tremendously in toxicity, and it is often trace pollutants that pose the greatest health risks.

The United States Environmental Protection Agency (US EPA) lists 189 toxic air pollutants in its revised Clean Air Act[1]. Of the 189 hazardous air pollutants (HAPs) or air toxics[2], approximately half are VOCs, with the balance comprising primarily metals, other inorganic compounds and semi-volatile organic compounds.

It is, however, very difficult to monitor concentrations of so many HAPs over large areas, and since the majority are traceable to particular sources (e.g., plastics or pesticide manufacture) there is little reason to monitor all 189 in all areas. Therefore the US EPA focused its attention on 33 HAPs that pose "the greatest threat to public health in the largest number of urban centers"[3]. Nineteen of these pollutants are VOCs. Since they pose such a widespread threat, it makes sense to routinely and widely monitor these VOCs in urban centers.

A key hindrance to wide-scale monitoring of even the urban HAPs is that an ideal technology (that is, one that is not only technically capable, but also practical and economical) has not been commercially available. Consequently, national environment agencies have targeted only the greatest threats to the wider population. For example:

- The National Air Quality Strategy (NAQS) for the United Kingdom[4] "sets objectives for eight air pollutants to protect health" (p7), of which two (benzene and 1,3-butadiene) are VOCs. Note that annual thresholds have been set for about 100 air pollutants (of which around half are VOCs)[5].
- The European Union directive 2008/50/EC seeking cleaner air for Europe[6] lists only one VOC: benzene.
- The New Zealand Ministry for the Environment's recently revised guidelines for air quality[7], added the "priority organic contaminants": benzene, 1,3-butadiene, formaldehyde and acetaldehyde. These VOCs are also indicated as most important by Australian authorities[8] and are the four major VOCs targeted in US air monitoring programs.

The remainder of this whitepaper briefly compares the most commonly available ambient monitoring technologies and then focuses on SIFT-MS, which provides a significant advance in real-time monitoring solution.

Technologies for real-time air quality monitoring

There are a number of commercially available technologies for continuous monitoring of ambient VOCs, several of which are compared in Table 1. Most techniques use some form of mass spectrometry, although the infrared spectroscopic technique is also popular.

Table 1 indicates that SIFT-MS offers the best fit for general, real-time VOC analysis in ambient air because it is easy to use, easily integrated, very sensitive and has high stability with respect to calibrations and humidity.

Table 1. A comparison of characteristics for several commercially available real-time and near real-time air quality monitoring technologies used for VOC analysis.[1]

Characteristic	Long-path FTIR	Fast GC/MS	MIMS	SRI-PTR-MS	SIFT-MS
Compounds accessible to technology	Wide	Wide, but limited by column	Wide, but limited by membrane	Wide	Wide
Selectivity	Moderate to high	High	Moderate	High	High
Limit of detection	10 ppbv	1 ppbv	1 ppbv	<1 pptv	<1 pptv
Accuracy	Moderate	High	Moderate	Moderate	High
Humidity effect	Significant	Significant	Minimal	Moderate	Minimal
Response time	Seconds	Several minutes	>10 s	100 ms	100 ms
Calibration frequency	Moderate	High	Moderate	Moderate	Low
Stability	Moderate	Moderate	Moderate	Moderate	High
Sample preparation	No	Sometimes	No	No	No
Required user skill level	High	Moderate to high	High	High	Caters to wide range of users
Software ease-of-use	Moderate	High	Moderate	Low	High
Remote operation	Yes	Yes	Yes	No	Yes
Maintenance	Moderate	High	Moderate	Moderate	Low

1 FTIR = Fourier Transform Infrared Spectroscopy; GC/MS = gas chromatography mass spectrometry; MIMS = membrane introduction mass spectrometry; SRI-PTR-MS = switchable reagent ion – proton transfer reaction mass spectrometry; SIFT-MS = selected ion flow tube mass spectrometry [9,10].

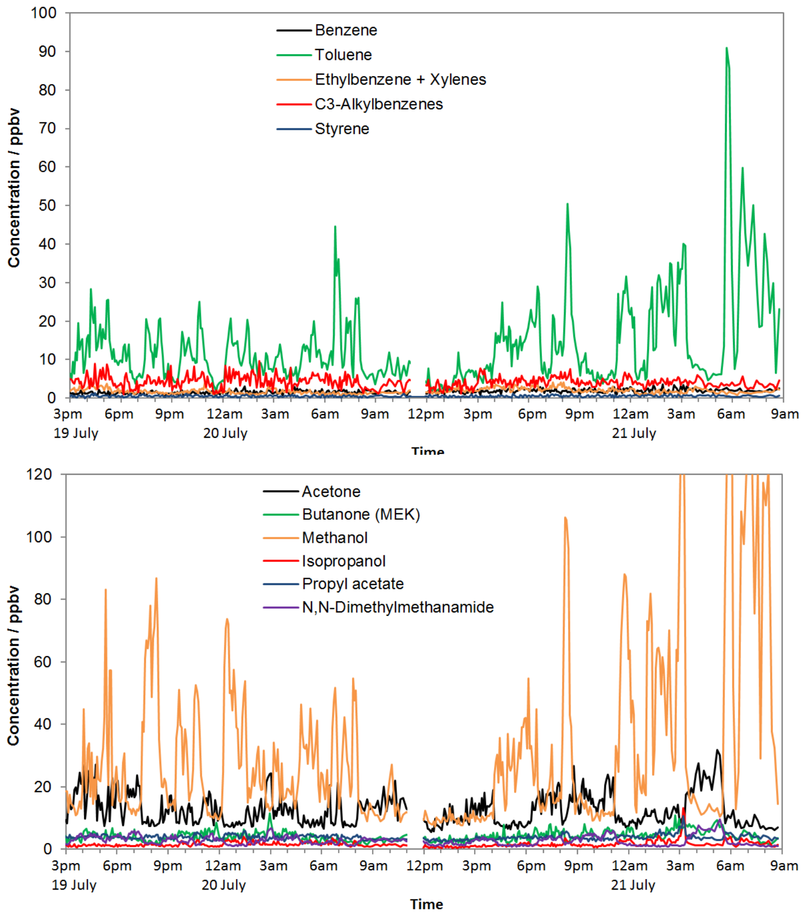
SIFT-MS measurement of HAPs

The high-speed analysis provided by SIFT-MS allows continuous monitoring of VOCs. Figure 1 shows concentration data obtained over a 42-hour period at a school adjacent to an industrial area near Taipei, Taiwan from 3pm on 19 July to 9am on 21 July 2011. The data for selected compounds were extracted from full mass scans acquired with five-minute time resolution.

Gusty wind conditions during the trial lead to increased signal variability compared to analysis in static air conditions. Nevertheless, several compounds show interesting trends over the sampling period, including toluene, C_3-alkylbenzenes (e.g. mesitylene), methanol, isopropyl alcohol, acetone and N,N-dimethylmethanamide.

The suitability of SIFT-MS for ambient air monitoring is, however, much greater than Figure 1 illustrates. SIFT-MS can analyze air for the vast majority of VOCs and is easily configured for analyzing different compounds. This means SIFT-MS can perform general air monitoring for a wide range of hazardous air pollutants or can be quickly configured to track compounds at a specific source. Table 2 lists some common air pollutants SIFT-MS can monitor in ambient air, together with national authorities that list them.

Figure 1. Concentrations (in ppbv) of selected compounds detected in ambient air, using SIFT-MS. The instrument was located in a school adjoining an industrial area near Taipei, Taiwan R.O.C.



Note:

1. Several brief analyses were undertaken during the one-hour period from 11am to 12pm on 20 July.
2. Data were not background corrected because there was no provision at the school site to make this measurement.
3. Concentration data were extracted from full mass scans, which allow detection of all reactive compounds. Selected ion mode (SIM) scans are also possible. SIM scans allow improved limits of detection and quantitation for selected (target) compounds.

Table 2. Some HAPs that can be routinely monitored using SIFT-MS. The number in square brackets refers to the reference.

HAP	US EPA Hazardous Air Pollutants[2]	UK DEFRA National Air Quality Strategy[4]	Australian National Pollutant Inventory[8]	New Zealand Ministry for the Environment[7]
benzene	•	•	•	•
toluene	•		•	
ethylbenzene + xylene isomers	•		•	
styrene	•		•	
formaldehyde	•		•	•
acetaldehyde	•		•	•
propionaldehyde	•			
acetone			•	
methanol			•	
ethanol			•	
n-hexane	•		•	
1,3-butadiene	•	•	•	•
hydrogen sulfide				•
nitrogen dioxide		•		•

Technical performance of the latest commercial SIFT-MS instruments in the ambient air monitoring application is described in reference 11.

Conclusion

VOCs are significant and widespread pollutants. Unfortunately the lack of an economical, real-time ambient air analysis technology has significantly limited widespread monitoring of hazardous VOCs in ambient air. SIFT-MS, a technology now being applied to ambient air monitoring, overcomes previous technological and practical limitations to provide a solution for monitoring volatile organic pollutants to pptv levels in real time. VOC-based air pollution incidents can now be detected and quantified in real time, and public exposure issues addressed.

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Syft Technologies Limited
3 Craft Place Middleton
PO Box 28149
Christchurch
New Zealand

Phone +64 3 338 6701
Fax +64 3 338 6704
Email sales@syft.com
Website **www.syft.com**