

EXTENDING SIFT-MS TO DETECTION OF SEMI-VOLATILES ON SURFACES

Daniel B. Milligan, Yan Li, John D.C. Gray, Barry J. Prince, Vaughan S. Langford, Murray J. McEwan
 Syft Technologies Limited, Christchurch, New Zealand
 Email: vaughan.langford@syft.com

Introduction

Selected Ion Flow Tube Mass Spectrometry (SIFT-MS) is a real-time analytical technique that detects volatile organic compounds (VOCs) and certain inorganic gases to low part-per-trillion concentrations (by volume; pptv) without sample preparation or preconcentration. These characteristics mean that SIFT-MS has traditionally been applied to real-time detection of VOCs in air.

The recent development of a swab desorber inlet has enabled SIFT-MS to be applied to detection of diverse semi-volatile organic compounds (SVOCs) swabbed from surfaces. In this study, we investigated the performance of swab-based SIFT-MS analysis of a variety of explosives, explosives taggants, drugs of abuse and their precursors, herbicides and pungent odour compounds.

Methods

SIFT-MS uses ultra-soft, precisely controlled chemical ionization coupled with mass spectrometric detection to rapidly quantify VOCs in gases to low part-per-trillion levels (by volume; pptv).

Three standard chemical ionization agents (reagent ions or precursor ions) are applied in SIFT-MS: H_3O^+ , NO^+ and O_2^+ . These reagent ions react with trace VOCs in very well controlled ion-molecule reactions but do not react with the major components of air, enabling SIFT-MS to analyze air for trace VOCs to low pptv levels without preconcentration. The reagent ions are switched within 10 milliseconds, providing unsurpassed selectivity among direct MS techniques. Figure 1 provides a schematic representation of the SIFT-MS technique.

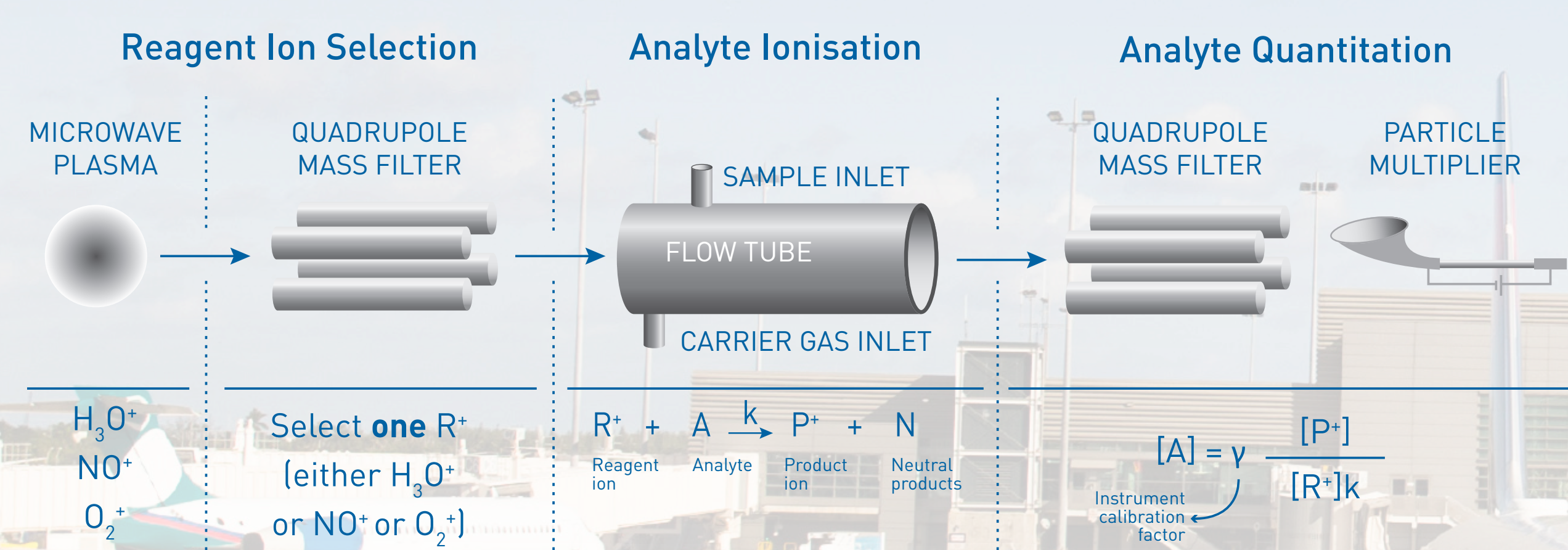


Figure 1. Schematic diagram of the SIFT-MS technique.

In order to extend SIFT-MS to detection of SVOCs, a swab desorber inlet has been developed for SIFT-MS. Figure 2 shows the concept of this inlet and the first-generation commercial product. The requirements for SIFT-MS differ significantly from those for GC/MS or ion mobility spectrometry (IMS) devices. For SIFT-MS, the SVOCs are desorbed into a 50-mL chamber prior to analysis, rather than applying flash desorption to form a very narrow pulse.

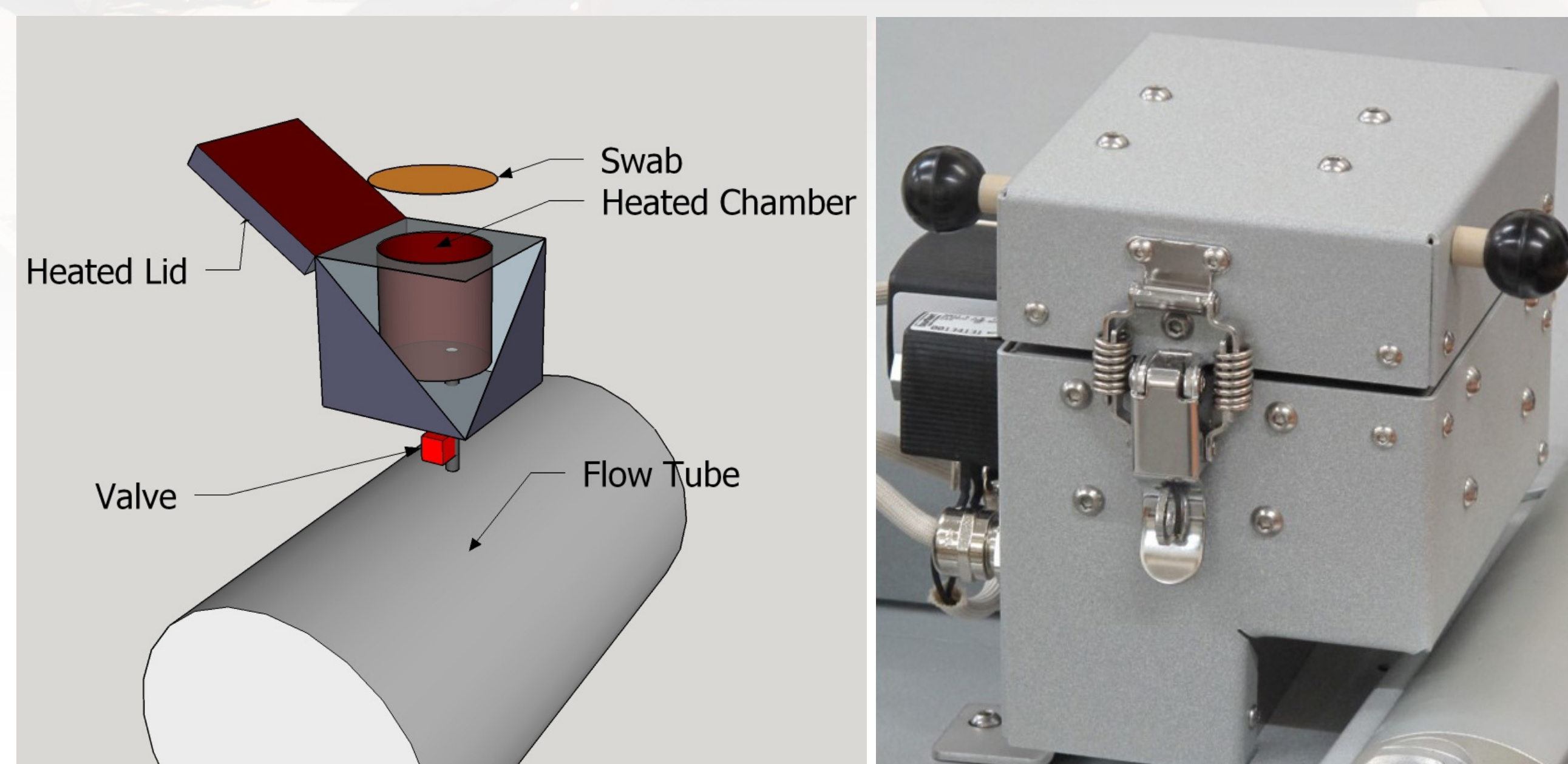


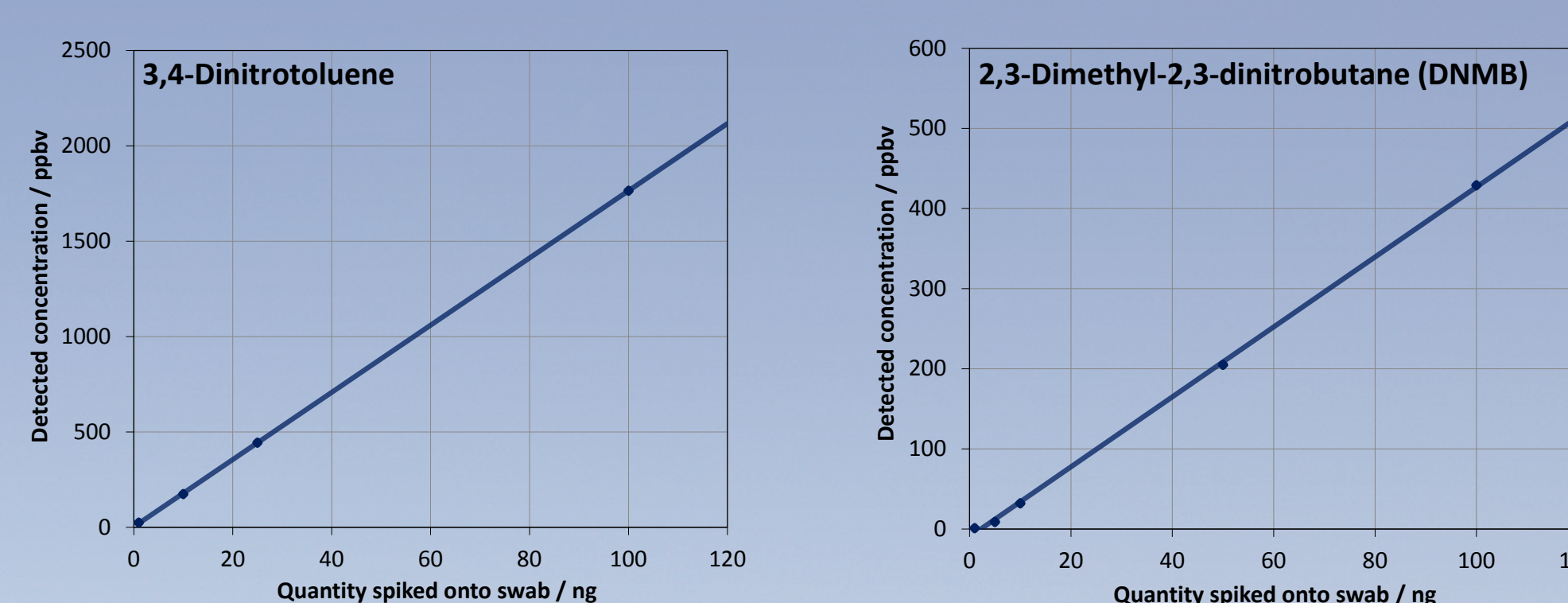
Figure 2: Concept design for a swab desorber inlet and the first-generation commercial product.

Serial dilutions of target compounds were prepared in dichloromethane and then spiked onto the swab. The dichloromethane solvent was evaporated at room temperature and then the swab was analysed using the swab desorber inlet and a Syft Technologies Voice200 SIFT-MS instrument.

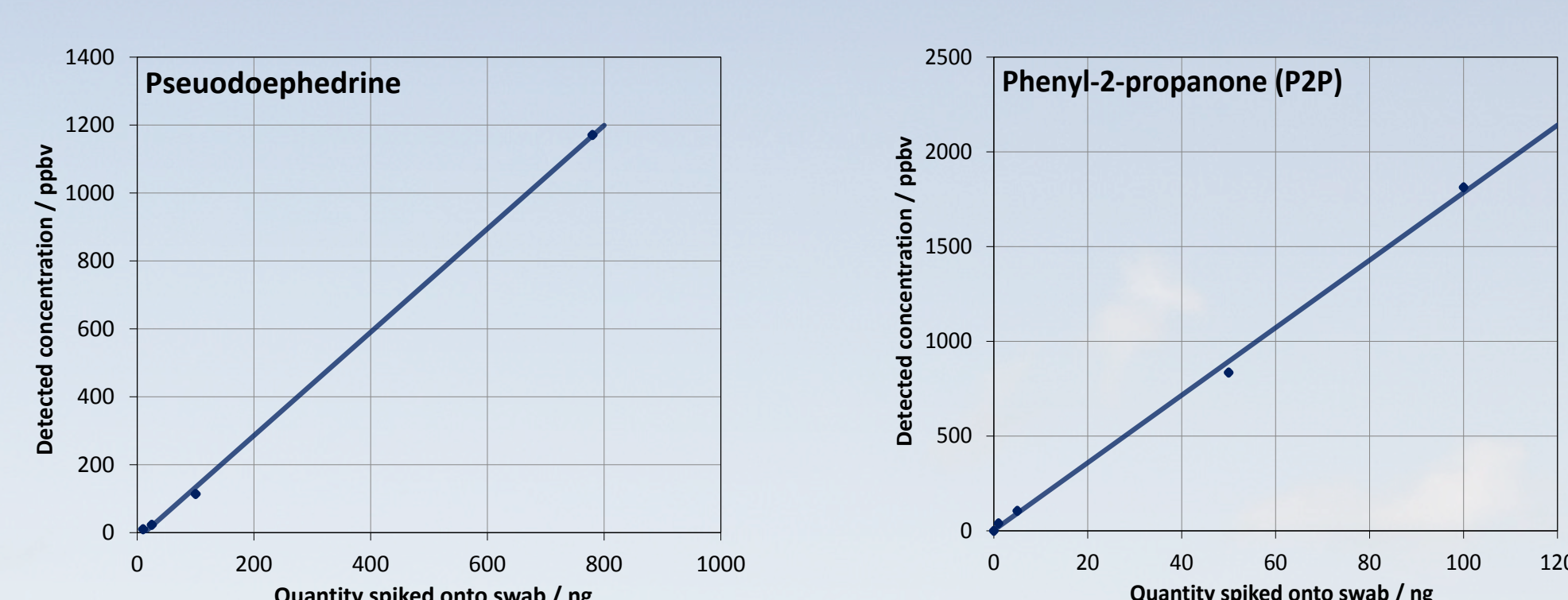
Results and Discussion

Linearity data for a variety of potential applications are shown below. Linear responses and detection limits in the low nanogram range are consistently observed, demonstrating potential for further development of SIFT-MS as a detection tool for SVOCs.

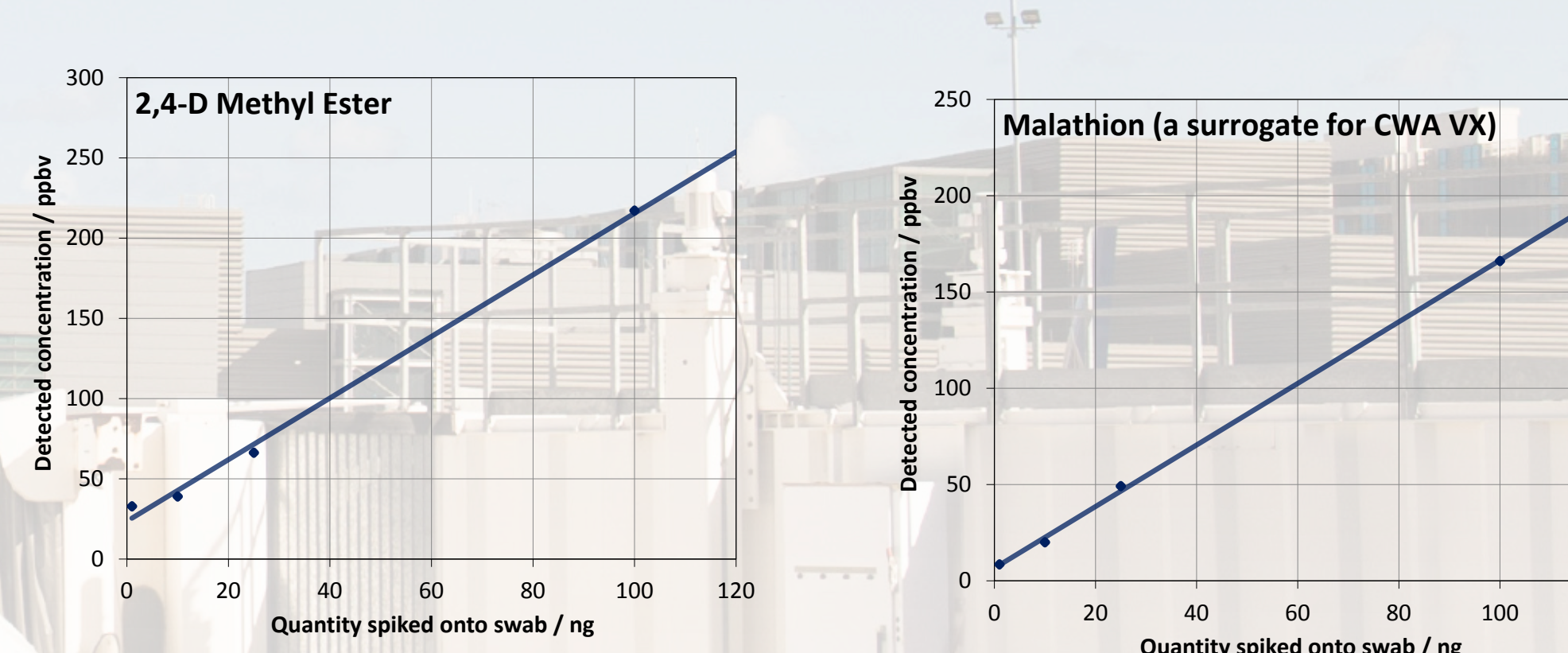
- Explosives and taggants:** for example, 2,4-dinitrotoluene and 2,3-dimethyl-2,3-dinitrobutane (DNMB).



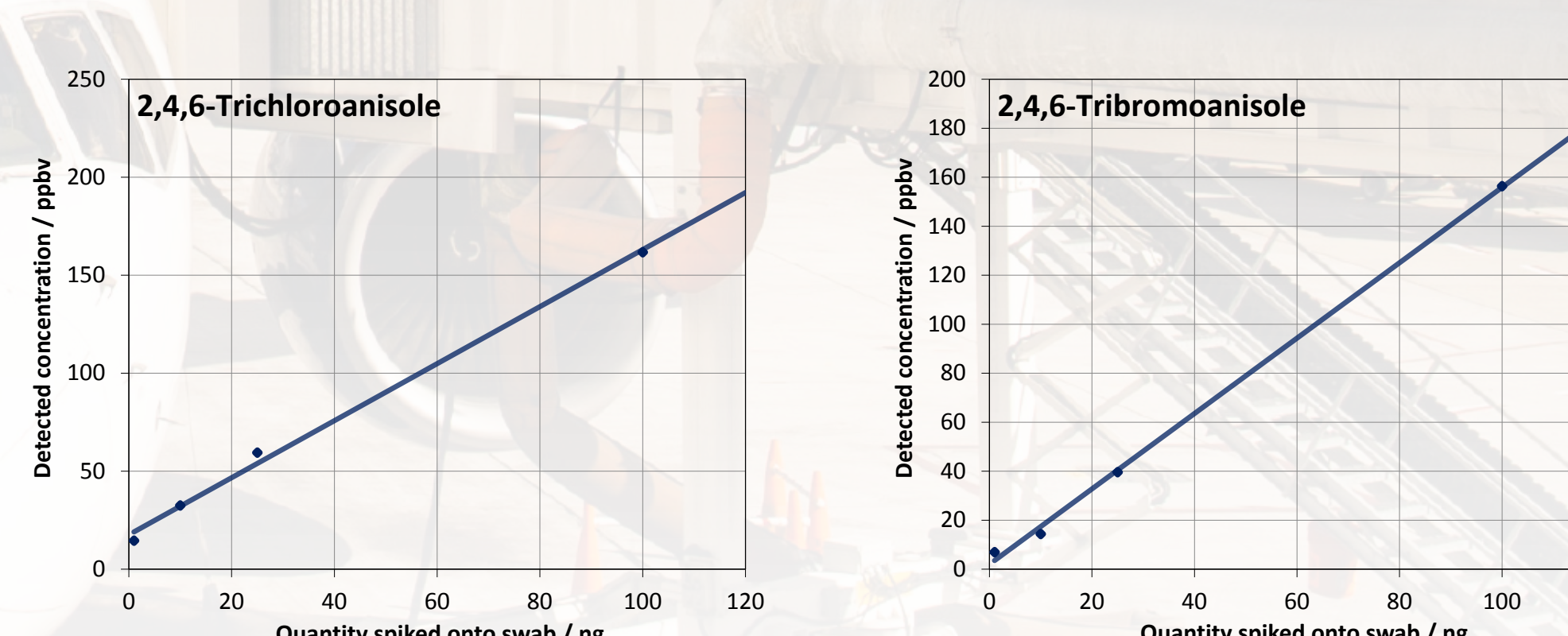
- Narcotics and precursors:** for example, pseudoephedrine and phenyl-2-propanone (P2P).



- Pesticides:** for example, 2,4-D methyl ester and malathion (which is also a surrogate for the chemical warfare agent (CWA) "VX")



- Food taint compounds:** for example, 2,4,6-trichloroanisole and 2,4,6-tribromoanisole.



Conclusions and Future Work

Very low nanogram quantities of SVOCs are readily detectable from swabs using SIFT-MS. SIFT-MS offers greater selectivity than IMS due to the combined application of three instantaneously switchable reagent ions (H_3O^+ , NO^+ and O_2^+) and mass spectrometric detection. This means that SIFT-MS provides unique opportunities for simple, rapid trace SVOC analysis in a variety of industries, including homeland security, customs agencies, and agriculture and food.

Future work will include evaluating the newly developed negatively charged reagent ion source for SIFT-MS. Negatively charged ions should provide even greater selectivity and, in the case of nitrated explosives, more sensitive detection.

References

- Prince, B.J., Milligan, D.B., & McEwan, M.J. (2010). *Rapid Commun. Mass Spectrom.*, 24, 1763-1769.
 Smith, D., & Spanel, P. (2005). *Mass Spec. Rev.*, 24, 661-700.