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Foreword

Harsh environment mass spectrometry: New developments and applications

The continuing development of micro- and nanofabrication technologies has allowed novel versions of miniature mass spectrometers and their component parts to become readily available. This has led to a number of miniature and field-portable instruments, which are finding increasing application in environments previously thought too difficult or too harsh for analysis. The selection of papers brought together in this special issue arose from the Harsh Environment Mass Spectrometry (HEMS) workshop held in Santa Barbara, California in September 2009. The HEMS workshop organizers are grateful to the Editors of IJMS for the opportunity to report on this work and draw the attention of the wider mass spectrometry (MS) community to some of the new developments in HEMS.

Instrument miniaturization is an important technology driver in this area, however not all papers in this issue report MS at the micro-scale. Some researchers use conventional mass spectrometers in field-portable systems. The common denominator in every case, however, is novel application in harsh environments. These can include active volcanoes, underwater environments, interplanetary space, and the battlefield. ULISSES is a small portable MS system for the study and visualization of gaseous volcanic emissions and is described in the article by Diaz et al. (University of Costa Rica) assisted by colleagues from NASA, JPL, ASRC and OTS. First deployments took place *in situ* to monitor the awakening of the Turrialba Volcano in Costa Rica. The cover photo of this Special Issue shows use of the ULISSES portable MS system at the active crater. Gas measurements were acquired prior and after the Turrialba eruption on January 5th 2010, confirming the presence of gas chemistry precursors typical of volcanic eruptions. Ground and airborne measurements represent a first step towards the use of unmanned aerial vehicles as future airborne platforms. In April 2010 the six-day shutdown of most European airports is estimated to have cost the airline industry at least $1.7 billion; in addition, millions of people suffered expense and inconvenience. MS-assisted early warning systems for impending volcanic activity and the chemical characterization of volcanic ash plumes represent an important and relevant HEMS application.

Following September 11, 2001, increased market demand has continued to drive development of small, rapid GC–MS systems. Reliable detection and identification of dangerous chemicals, including chemical warfare agent (CWA) analytes is important to protect military forces and for public safety, and GC–MS is well suited for this application. Smith et al. from the Uniformed Services University (Maryland), and colleagues from Defence R&D Canada-Suffield and BYU (Utah) describe use of two field-portable GC–MS systems for CWA detection. The CWA O-ethyl-S-2-diisopropylaminoethyl methylphosphonothiolate (VX) and its many degradation products are challenging GC–MS analytes for a transmission quadrupole detector; however, use of mass spectra and retention index information resulted in accurate identification of VX and related analytes. Interesting ion/molecule chemistry was also observed with analysis of volatile nerve agents such as O-isopropyl methylphosphonofluoridate (Sarin) using a small cylindrical ion trap detector.

Lauritsen and Neilsen from the University of Copenhagen report on their use of hot cell membrane inlet mass spectrometry (MIMS) where a solid sample can be analyzed for its potential liberation of hydrophobic organic compounds directly and without pre-treatment. The application envisaged is usage in paramedical vehicles for immediate, on-site identification of medication found near intoxicated patients. Results using the technique demonstrate that the active ingredient in many common tablets such as anti depressives, pain relievers, epileptic medicine, and antihistamines, are recognized directly and without pre-treatment.

Some have suggested that interplanetary space is the ultimate harsh environment. Getty and co-workers at NASA Goddard, University of Maryland Baltimore County, Bastion Technologies, and Honeybee Robotics report on the development of VAPoR, a pyrolysis oven and a miniature ToF-MS for use in mass- and power-constrained planetary science missions to study the mineralogy and geochemistry of planetary surfaces. The VAPoR prototype, in both laboratory and field-testing, demonstrated characterization of analog samples relevant to planetary science, including volcanic rock samples from Mauna Kea in Hawaii.

As in previous HEMS workshops novel forms of MS instruments were reported. Brucker and Rathbone from Brooks Automation describe a novel electrostatic ion trap, which uses anharmonic resonant trapping. Unlimited mass range, good sensitivity at high and ultrahigh vacuum levels, small size, low power requirements, and compact construction are reported. Fast mass spectra data acquisition rates allow applications from fast moving platforms (e.g. aerospace). Manard and co-workers at National Security Technologies and Sionex present the design of a prototype, field-portable MS system with an atmospheric interface devised to couple directly to a differential mobility mass spectrometry (DMS) unit. Applications have found that DMS is effective in reducing chemical noise, separating isobaric ions and charge states, achieving rapid analysis, and improving the accuracy of quantitative measurements in complex samples.

In the final three papers the focus is on miniaturization. Reinhardt and colleagues at the TUHH (Hamburg) report on their planar integrated micro mass spectrometer (PIMMS), which shifts the

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lower limit of the measurable mass spectrum from 12 to 3 Da. This mass shift was achieved by doubling the size of the finger electrodes of the synchronous ion shield (SIS) mass analyzer from 800 to 1600 μm; detection of helium allows the use of PIMMS for helium leak detection applications. The installation of a micro channel plate improves the sensitivity of the instrument to <400 ppm. Jesseph et al. at the University of North Texas present data taken from a 0.5 mm r_0 cylindrical ion trap tracking the performance during storage and tandem experiments using xylene. Isolation of the precursor ion was accomplished by modulating the DC ramp voltage, and collision-induced dissociation was accomplished by applying various tickle voltages to the end-caps of the ion trap. From the results obtained, the projected performance of smaller ion traps (down to approximately 1 μm) was considered. Austin et al. from BYU (Utah) describe ion trap mass analyzers constructed from arrays of independent electrodes, which may also be microfabricated. Such arrangements allow unprecedented control and variability of electric field shapes. With ion traps made using two opposing electrode array plates, both even- and odd-order multipoles can be independently adjusted, which are known to affect ion trapping and mass analysis characteristics in quadrupole ion traps.

In summary, the contributions in this IJMS Special Issue reflect ongoing high quality research into miniature and portable mass spectrometry in harsh environments and in field conditions. There is little doubt that further developments in this area will see the emergence of novel instruments with improved characteristics, leading to further exciting applications. The 8th HEMS workshop is scheduled for the fall of 2011. All interested are most welcome either as attendees or better still as participants. Details will be announced on the website (http://www.hems-workshop.org), which also carries copies of papers and posters presented at previous workshops.

Stephen Taylor[1]
Department of Electrical Engineering and Electronics, University of Liverpool, Liverpool, UK

Guest Editor
Veronica M. Bierbaum*
Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO, USA

* Corresponding author.
E-mail address: veronica.bierbaum@colorado.edu (V.M. Bierbaum)

[1] 7th HEMS Workshop Committee Member.

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