Recent advances and development trends in miniature mass spectrometry

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In today's world, we face new and increasingly complex chemical challenges at multiple levels. There are security, environmental and healthcare challenges with short and/or long term consequences. This has led to the need for real time, accurate chemical analysis in the field (outside of the laboratory). This in turn has led to a growing trend in the area of instrument miniaturization. Recent advances in the conception, design, integration, optimization and use of miniature and portable analytical instruments allows development of 'field laboratories' for a wide range of application areas including environmental, medical, security, quality assurance, planetary exploration, etc. The purpose of this special issue is to provide a brief survey of the current state of the instrumentation through papers by some of the key players.

Among the technologies and instruments available for *in-situ* operations, mass spectrometers (MS) and ion mobility spectrometers (IMS) are analytical instruments of choice for in situ chemical analysis, allowing the simultaneous determination of qualitative, quantitative and structural information. The knowledge resulting from this information assists and enhances the process of effective decision-making at the point of analysis (PoA). Mass spectrometry, as a leading and well established analytical technique, presents numerous advantageous characteristics in the chemical investigation (detection, monitoring, profiling, fingerprinting, mapping, etc.) of harsh environments. It offers superior levels of high sensitivity, very low detection limits, rapid response times and wide range of molecular applicability (organic, inorganic, volatile, non-volatile, etc.) allowing the characterization of small, large, single-analyte and complicated mixtures.

The instruments discussed in this special issue have developed to address several important questions. The Verbeck group at the University of North Texas in collaboration with Inficon Inc. report the integration, testing and validation of a portable membrane inlet mass spectrometer (MIMS) for the on-site analysis of environmental pollutants. Their work focuses on the detection and monitoring of anthropogenic volatile organic compounds

(VOCs) with special emphasis in BTEX in aqueous and air samples. Results from multiple sites in the sub-Antarctic region of Puerto Williams, Chile are presented and discussed. Their MIMS system is coupled with a GPS to enhance the chemical data by providing simultaneous spatial and temporal results. The majority of analytes associated with applications in harsh environments e.g. for search and rescue operations and homeland security (narcotics, explosives, chemical and biological weapons), have molecular weights below 1000 Da. However, in some cases, there is the need to monitor larger chemical compounds with complicated structures and physical and chemical properties. To achieve this, maintaining at the same time the power requirements in low levels (which is highly desirable for fieldable systems), innovative application of the fundamental physical principles are required. Graham Cooks laboratory in Purdue University (Aston Laboratories) propose an alternative approach to increase instrument mass range based on scanning of the resonance ejection frequency in a non-linear fashion using an inverse Mathieu q scan. Experiments with both a laboratory based commercial instrument (Thermo LTQ) and a built-in-house miniature ion trap MS (Mini 12) have confirmed the above concept. Results obtained showed an impressive increase in mass range in both cases (2.5x for the LTQ and 3.5x for the Mini 12) compared to traditional existing approaches used currently for mass range extension. It is noteworthy that the novel methodology demonstrated a respectable enhancement of the analytical capabilities of the systems used without instrumental modifications.

There are two papers in the current issue which investigate the development and testing of micro-engineered MS components. The first article explores a miniature electron ionization source, and the second one deals with a new generation of micro-fabricated time-of-flight MS (μ-ToF MS). Micro-Electro-Mechanical Systems (MEMS) continue to be developed and remain of high scientific interest. The challenge for these approaches is to maintain their high performance analytical characteristics at the same time as reducing the overall instrument size. Researchers from Duke University report on the design, simulation, fabrication and experimental characterization of a novel MEMS electron ionization source with integrated carbon nanotube (CNT) field emission cathodes and a low-temperature co-fired ceramic (LTCC) carrier. The miniaturized ion source was manufactured using the Polysilicon Multi-User MEMS Process (PolyMUMP), optimised with SIMION software and evaluated experimentally with a range of chemical analytes. On the other hand, research

work undertaken in the Alternative Energies and Atomic Energy Commission (CEA) in France on a MEMS μ-ToF MS system showed that significant progress has been achieved towards future pocket size systems (stand-alone MS or hybrid) for gas analysis. Experimental mass spectra of alkanes (C1 to C6) gas mixtures demonstrated detection limits below 100 ppm.
A unique, compact, low power and state-of-the-art, dual-source, linear ion trap (LIT) MS capable of pyrolysis-gas chromatography MS (pyr/ GC-MS) and laser desorption/ionization MS (LDI-MS) is the basic instrument being developed for the ExoMars Rover which will investigate the Martian environment. The mission will investigate and perform in-situ analysis of the Martian atmosphere and soil in the search for biological and other molecules necessary to sustain life. This work is also relevant to future planetary missions. The system under development will also attempt mineralogical analysis to detect refractory organic compounds. Tandem MS (MS/MS) capability will enhance the in-situ chemical analysis and provide an additional stage of molecular confirmation. Smart, automated sampling techniques have been already been developed to address the specific challenges of the harsh Martian environment.

Costanzo et al. from Breathtec Biomedical Inc. in collaboration with Cannabix Technologies Inc. and the Yost group from the University of Florida describe the current status and future perspectives in the area of Field Asymmetric Ion Mobility Spectrometry (FAIMS). Their article presents the use of FAIMS devices in the area of law enforcement, and in environmental screening of pesticides, insecticides and other toxic pollutants hazardous to human life. FAIMS is also being investigated in the biomedical world as a non-invasive, diagnostic tool for the rapid detection and monitoring of disease biomarkers via breath analysis. FAIMS based systems have great potential in field applications due to their overall size, low maintenance costs and operational simplicity. This special issue closes with a paper from Fedele et al. which investigates the use of portable mass spectrometry in the monitoring of geophysical and geochemical phenomena. Specifically, the article presents the on-line screening of magmatic and hydrothermal gaseous emissions (CO_2/H_2S, H_2S/H_2, He/CO_2, CH_4/CO_2) released from the unsteady fumaroles of the Pisciarelli area in South Italy in 2009 and 2012. The described system and the followed operational approach enable to carefully ‘listen to’ the sounds of our planet. MS was proved an excellent tool for sampling and analysing gases related to volcanic activities and potentially could be used to predict earthquakes or other physical catastrophes.

Undoubtedly, significant technological progress in the area of miniature MS systems has been achieved in the last few decades. Miniature and portable MS and IMS systems continue to be developed as universal analytical tools for *in-situ* chemical analysis inside and outside the laboratory.