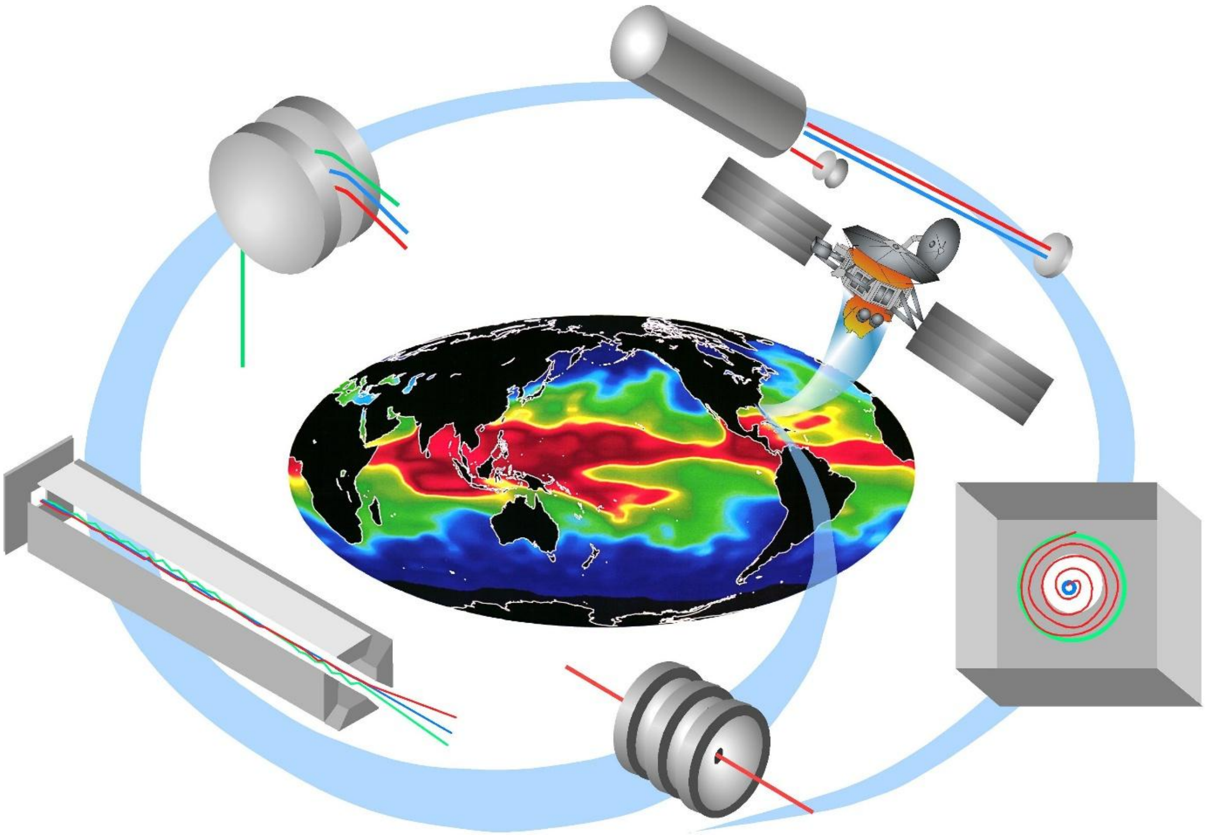
2025 HEMS WS Abstracts in Order of Oral Presentations in Program



Using Classes of Molecules to Identify Air Health

Dr. Guido Verbeck - United States - Augusta University

Abstract

Chemical releases, whether intentional or accidental, can be hazards to people's health, both from airborne contaminants from system failures, as well as chemical metabolites from unhealthy individuals. Discrete classes of compounds and mixtures can be used to identify certain hazards in the air. Examples are BTEXs from oil and fuel leaks, organophosphate in chemical weapons, to metabolites from unhealthy individuals (i.e., ketones and aldehydes from respiratory distress, unsaturated hydrocarbons and aromatics from bacterial infections). Because of the complex nature of the environment, isolation of specific classes of compounds from the surrounding matrix can aid in making quick assessment as to the overall quality of the health of the environment. Here we introduce the concept of combining different substrate capture with membrane inlet to create a make-shift fast separation technique for rapid analysis. This is performed by dividing the cabin air into specific capture substrates based on chemical class, and then introducing these events into a highly sensitive and selective portable mass spectrometer. This novel instrument can sample and respond is real-time with less than a 15 second delay.

Biography - Guido Verbeck

Dr. Guido F. Verbeck, Chair and Professor of Chemistry and Biochemistry, is an expert is mass spectrometry, specifically instrument design and development. Dr. Verbeck received his PhD as a Proctor & Gamble fellow in chemistry at Texas A&M University. Dr. Verbeck has developed mass spectrometers and chemical instruments over the past 24 years, and has been a member of the analytical community for 28 years. His appointment is at the Augusta University where he continues to design novel ion optical devices for miniaturization, preparative, and analytical mass spectrometry, and is the Director for the Laboratory of Imaging Mass Spectrometry.

Keywords

Mass spectrometry, Air quality, VOCs, Fieldable

ARAMMIS: Autonomous Robots for Area Mapping, Monitoring and In-situ gas Sensing, focused on Lunar exploration and Earth Science applications

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Dr. James Fox - United States - INFICON ISS Emerging Technologies and New Markets Research Group
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Abstract

The ARAMMIS project is a collaborative research effort between INFICON and ETH Zurich's Robotic Systems Lab (RSL) to develop and deploy autonomous robots enabled with gas sensing capabilities to provide 3D gas concentration mapping, monitoring, and in-situ sampling of varied environments, especially focused on Earth Science geochemical applications and Lunar analog demonstration for future Space exploration missions.

A commercially available, compact quadrupole mass spectrometer-based system has been mechanically and electrically integrated into a legged robot. The overall system, named **ARAMMIS** (**A**utonomous **R**obot for **A**rea **M**apping, **M**onitoring and **I**n-situ gas **S**ensing), is designed for deployment in diverse environments such as chemical plants, oil installations, semiconductor factories, as well as open fields, geological sites, caves, volcanoes, and even emergency scenarios. Its purpose is to map gas concentrations across the area or locate gas sources where concentrations exceed the background levels. The MS operating commands and data retrieval are carried out fully autonomously through the robot’s main computer.

The first volcano deployment of the ARAMMIS system using the Transpector MPH quadrupole mass spectrometer, integrated into RSL's modified ANYmal D legged robot, was performed in June 2025 at Mt Etna volcano´s Cratere del Laghetto (an established ESA and NASA Lunar analog site), in collaboration with INGV Rome, Palermo, and Catania groups, the University of Costa Rica, University of Pisa, and University of Catania.

The mission objective was to test the autonomous capabilities of the ARAMMIS robot by walking at the rim of an active crater to characterize the emitted gases, enabling in-situ real-time analysis together with other robotic platforms and gas sensing instruments. These experiments support geochemical Earth sciences by contributing to volcano gas emission studies aimed at establishing eruption precursors, while also demonstrating capabilities relevant to future lunar exploration in terrains with similar characteristics.

Biography - James Fox

Dr. James Fox is a Staff Research Scientist at INFICON with more than 12 yrs experience in mass spectrometer design, testing , integration and applications. He earned his bachelor's degree in chemistry at Sam Houston State University in Huntsville, TX. From there, he attended the University of North Texas, earning a doctorate in analytical chemistry with a research background in mass spectrometry theory, design and applications. In 2013, he joined INFICON Inc. in East Syracuse, NY where he is part of the Emerging Technologies and New Markets research application group.

Keywords

Robotic Platforms, Earth Science, Lunar Analog, Exploration, Volcano gas detection and monitoring

A cart-portable TOF-MS coupled with a thermal desorber for in-field analysis of CBRNE threat materials

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Mr. David Thompson - Canada - Canadian Nuclear Laboratories
Dr. Ankur Chaudhuri - Canada - Canadian Nuclear Laboratories
Dr. Mayra Martinez - Canada - Canadian Nuclear Laboratories
Dr. Thomas Domingo - Canada - Canadian Nuclear Laboratories
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Abstract

A field-deployable mass spectrometer (MS) would provide first responders and law enforcement with a portable tool for rapid and accurate identification of chemical, biological, radiological, nuclear, or explosive (CBRNE) threats. It would provide preliminary field data to both guide the best course of action and focus any subsequent forensics analysis. CNL is developing a cart-portable high-resolution time-of-flight MS (portable TOF-MS) system that can be rapidly deployed for in-field measurements. The equipment consists of a commercial off-the-shelf compact multi-turn TOF-MS weighing 40 kg and housed in a robust shock-absorbing cart with an onboard UPS that allows for hours of self-powered operation. The capability of portable TOF-MS in measurement of gas samples has been tested. Measured Xe, Kr, and Ar isotopic compositions demonstrated its ability to reproducibly detect and quantify isotope ratios of the gas samples in different atmospheric conditions, ranging from indoor laboratory conditions to outdoor field conditions. For liquid samples, dissolved organic compounds were directly introduced into the TOF-MS electron ionization source and successfully detected. However, by introducing analytes in this manner the system suffered from memory effects, clogging and loss of vacuum.

The sample introduction of the system was further modified externally to accommodate more sample types and enable rapid in-field sampling. A commercially available thermal desorber (TD) unit was coupled to the ionization source through a custom transfer-line. The coupling of TD and TOF-MS into a congruent functional TD-TOF-MS system was successful. Using a sample tube, controlled amounts of samples can be loaded into the TD. The sample tube is heated in a flow of carrier gas and desorbed analytes are swept into an electrically cooled focusing trap. The focusing trap is then heated rapidly in a reverse flow of carrier gas to transfer neutral analytes into ionization source. The TD-TOF-MS offers a system that could rapidly evolve analytes from samples followed by field measurements. Current testing of the TD-TOF-MS system with calibration standards and organic samples indicate the system's potential for measurements of an array of sample types, though some materials may need to be derivatized to increase their volatility to allow for desorption. Further optimization in the lab will be followed by field testing campaign of CBRNE samples. The current progress towards development of this field-deployable mass spectrometer will be presented.

This work is funded under Atomic Energy of Canada Limited's Federal Nuclear Science and Technology Work Plan.

Biography - Bett Kimutai

Bett Kimutai has a background in analytical chemistry and biochemistry. He received his PhD from Wayne State University in 2019. He initially worked as an analytical chemist in a diagnostic and drug testing lab. In 2023, he joined the nuclear response and analysis branch at Canadian Nuclear Laboratories. As part of the nuclear forensics team, he has roles in advancing nuclear forensics capabilities for investigation of nuclear and radiological materials. Some of his projects develop methodologies for characterization of nuclear and radiological materials using ICP-MS and develop field deployable capabilities for detection of CBRNE using portable TOF-MS.

Keywords

Portable, TOF-MS, Desorption, Field-deployable

Spaceflight Laser Desorption Orbitrap Mass Spectrometry

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Dr. Oya Kawashima - United States - University of Maryland, College Park, Institute of Space and Astronautical Science, JAXA
Mr. Lucas Andrews - United States - University of Maryland, College Park
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Prof. Ricardo Arevalo - United States - University of Maryland, College Park

Abstract

Laser Desorption Mass Spectrometry (LDMS) is an analytical technique commonly applied for measuring the chemical composition of solid materials. Advantages of LDMS include: spatially resolved measurements, enabling 2D chemical mapping; analysis of inorganic and organic compounds, providing context for detected biomarkers; and rapid experimental cadence, maximizing duty cycle. LDMS instrumentation has been developed for harsh environments, such as the surface of Mars (via the Mars Organic Molecule Analyzer – MOMA (*1*)), Titan (via the Dragonfly Mass Spectrometer – DraMS (*2*)), and the Moon (via the laser-based mass spectrometry – LIMS (*3*)). These systems, however, rely on linear ion traps or time-of-flight mass analyzers that can struggle to resolve spectral interferences. In comparison, next-generation LDMS instruments that leverage ultrahigh resolution analyzers, like the Orbitrap^{TM}, have the capacity to resolve spectral interferences (e.g. CO_2 and ^{44}Ca, or ^{54}Cr and ^{54}Fe) expanding access to a wider range of elemental, isotopic, and molecular measurements.

The Characterization of Ocean Residues and Life Signatures (CORALS) (*4*) and Characterizing Regolith And Trace Economic Resources (CRATER) (*5*) instruments are two LDMS instruments centered around an Orbitrap mass analyzer and designed for exploration of ocean worlds and the lunar surface respectively. Both investigations require approximately 10 kg of mass and less than 60 W of peak power facilitating accommodation on a wide range of spacecraft. Initial testing of these instruments (and earlier proof-of-concept prototypes) were focused on the detection of organic compounds at abundances higher than those expected in most planetary materials (e.g., wt.% levels of amino acids (*6*)) and measurements of trace element abundances in synthetic materials with unnatural major element compositions (e.g., rare earth elements in NIST SRM610 (*7*). More recently, performance testing of CORALS/CRATER has extended to isotopic ratios with permil level precision, quantification of elemental abundances in geologic materials to within 10% of true values, chemical mapping of meteorites, quantification of modal abundances of mineralogy via chemical mapping, training of machine learning models to classify mineralogy, and distinguishing biotic and abiotic sources. Here, I will review the most recent results collected from these protoflight and relevant commercial analog systems and discuss applications beyond planetary science.

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Biography - Madeline Raith

I am a PhD candidate at the University of Maryland, College Park studying Geology. My primary research topics are developing spaceflight laser based mass spectrometry to conduct quantification of elemental abundances in geologic material, understanding why minerals affect organic detectability via laser desorption mass spectrometry (LDMS), and characterizing native organic distributions in Mars analog samples.

Keywords

Laser Desorption, Orbitrap, Geochemistry, Astrobiology

A rugged and field deployable multi-laser resonance Single Particle Mass Spectrometer: Ship-based detection of trace metal-containing aerosols in the atmosphere of the Indian Ocean

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Abstract

A newly developed aerosol Single-Particle Mass Spectrometer (SPMS) employs advanced resonant laser ionization processes, enabling highly sensitive detection of transition metals (Passig et al., 2020) and organic molecules, such as polycyclic aromatic hydrocarbons (Schade et al., 2019). The technology, however, uses three laser pulses for laser desorption (IR laser), Resonance-Enhanced Multi-Photon Ionization (REMPI) of organic molecules (UV laser) and Laser/Desorption Ionization (LDI) with focused UV-laser pulses (i.e., plasma ionization). By using a back-reflection and re-focusing concept both ionization processes (LDI and REMPI) could be performed by the same laser (Schade et al., 2019). This development paved the way to develop a compact and rugged SPMS system, which now can be deployed to remote areas (e.g., high-altitude mountain stations) or on long cruises aboard on research vessels. Here we present preliminary data from particle-resolved measurements during a ship cruise with research vessel RV SONNE across the Indian Ocean in late 2024 in the framework of the GEOTRACES project. Atmospheric aerosol deposition is an important source of iron and other essential micronutrients in open ocean regions where their scarcity limits primary production, influencing marine ecosystems and oceanic carbon sequestration (Mahowald et al., 2018). In general, desert dust is the dominant source of trace metals by mass, but their bioavailability in dust is very low. Anthropogenic sources release e.g., pyrogenic iron with higher bioavailability, and these emissions are believed to be an important source of aerosol micronutrients in many regions. Significant uncertainties arise due to the lack of methods for assessing metal solubility at low aerosol concentrations and the scarcity of field data. Throughout the cruise, the new SPMS unit analyzed hundreds of thousands of individual particles. While sea salt aerosol was the dominant particle class, thousands of Fe-containing particles from long-range transport were also detected. Among them were numerous transition-metal-rich particles from mining activities in Australia, observed in the open ocean several hundred kilometers off the coast (see Fig. 1). Most metal-containing particles showed a high variability in the composition of secondary particle components, indicating different sources, transport pathways and aging mechanisms. Since the SPMS detects internal mixtures of trace metals with solubility-modulating components such as chlorine, sulfate, or dicarboxylic acids, it proves highly suitable for assessing particle sources and

the bioavailability of contained metals. In general, the measurements in this sparsely investigated region showed a surprisingly high contribution of anthropogenic sources to iron-containing aerosol in relation to desert dust, highlighting a potentially underestimated pathway in biogeochemical cycles. Finally, we have demonstrated that the newly developed SPMS unit is ruggedized enough to be applicable for months-long ship-based measurement campaigns in rough seas.

We gratefully acknowledge funding for RV SONNE ship-time (SO308) by the German Federal Ministry of Education and Research (BMBF), project number 03G0308A. Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - SFB 1477 “Light-Matter Interactions at Interfaces”, project number 441234705.

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Biography - Aleksandrs Kalamasnikovs

I am a PhD student at the University of Rostock in Germany, working towards a degree in Natural Sciences. Prior to studying in Rostock, I graduated from Riga Technical University in Latvia with a Bachelor's and Master's degree in Environmental Science. My current research focuses on developing novel real-time techniques for the physical and chemical characterization of ambient aerosols. Day-to-day, I mostly work with Single Particle Mass Spectrometers in various configurations and environments, for the non-destructive laser desorption of molecules.

Keywords

Marine aerosols, Single particle mass spectrometry, Indian Ocean, Long-range transport, Ship-based

Non-proximate, Handheld Probe with Positional Feedback for Real-time Analysis of Three-dimensional Object Surfaces

Dr. G. Asher Newsome - United States - Smithsonian Museum Conservation Institute

Abstract

Non-proximate desorption photoionization mass spectrometry (NPDPI-MS) was recently designed to analyze large, intact objects whose bulk requires positioning far from the instrument inlet. The first system used a rigid transport tube and detached, heated gas jet probe to identify dyes, plasticizers, and other organic molecules from convex surfaces ≥1 meter across. Neutral desorbed analytes were transported to a custom photoionization system. The rigidity of the transfer tube, however, required that the object be positioned in the desorption zone with sub-millimeter precision: a slow and unwieldy process when analyzing a large artwork or cultural heritage item. A new, flexible transfer tube design is implemented here to make analysis faster and more versatile. The 2-4 m transfer line is based on custom gooseneck tubing which satisfies multiple requirements: flexibility; stainless steel construction with inert coating; heating to minimize adsorption; and large inner diameter for analyte collection and carryover purging. An integrated desorption/suction probe suitable for manual use is built around the non-proximate end of the transfer line. The probe can be used on objects one-handed, while the other hand operates an integrated control module.

The sampling probe is designed for maximum efficiency, collecting desorbed analyte without loss so that heat exposure to a sample surface is minimized. A shaped inlet attachment slides along the end of the transfer line terminal, indicating by LED when the probe is in optimal position. Piezo sensors arrayed around the probe also signal physical contact, helping the user to avoid inner walls when probing inside a concave object. When the positioning is satisfactory, the user triggers a pulse from a 190 °C, 1 L/min nitrogen jet to desorb analyte from a 9 mm^2 area. Desorbed analyte is drawn into the transfer line at 4.8 L/min, where it is doped with anisole by an in-line permeation device and ionized in real time.

Irregularly-shaped objects on a stationary tabletop were sampled for demonstration purposes without moving them, using extractive solvent, or causing discernable physical damage. Caffeine was observed from a coffee stain at the base of an intact coffee mug; multiple compounds were observed from food paste residue at the bottom on an even deeper clay pot. Peppermint gum flavoring agents were observed from the semi-rigid rubber sole in between the cleats of an athletic shoe. The probe was also adjusted for analysis without pressing against a surface to sample from the soft surface of a citrus fruit. When analyte signal persisted after the gas jet pulse, the flow system was purged at 20 L/min to return to baseline signal levels.

Biography - G. Asher Newsome

G. Asher Newsome is a Physical Scientist and mass spectrometrist at the Smithsonian Museum Conservation Institute. Much of his current research involves developing ambient sampling techniques for cultural heritage and conservation science applications, with a particular interest in analyzing intact objects too precious for micro-sectioning, too fragile to be moved to the laboratory, too large to be positioned immediately adjacent to a typical mass spectrometer, and/or with other complex requirements. He frequently works closely with curators, conservators, and cultural representatives to determine an acceptable level of “invasiveness” for analysis. He holds a PhD in Analytical Chemistry from UNC-Chapel Hill.

Keywords

Photoionization, Thermal desorption, Accessibility, Practicality

2D MS/MS using Quadrupole Ion Trap Mass Spectrometry

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Mr. Thomas C. Sams - United States - Dept of Chemistry, Purdue University, 560 Oval Drive, West Lafayette, IN 47907

Dr. Edwin Gonzalez - United States - Teledyne FLIR Detection

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Abstract

The complexity of samples collected and analyzed outside of the laboratory is compounded by the lack of sophisticated sample clean up available in the field. One solution to this problem is use of a miniature fieldable mass spectrometer with ambient ionization. Such an instrument can provide chemically specific information for a wide range of sample types and matrix diversity with minimum to no sample clean up. 2D MS/MS is a scanning method implemented on ion traps which provides complete tandem mass spectrometric information on all ions generated from the sample. A spectrum is recorded in about a second while fragmenting each precursor ion using a supplementary ac frequency applied in the x-direction and then another much faster ac frequency scan for product ion ejection in the orthogonal y-direction. The additional dimension of information lends itself well to field-collected samples of a variety of types, including plant extracts, chemical reaction mixtures and drugs in biofluids. The 2D spectra are displayed so that for every precursor ion on the x-axis, the resultant product ions are displayed on the y-axis. 2D MS/MS can be used to identify classes of molecules through similar fragmentation patterns, especially by constant neutral loss signals which appear as diagonals, and precursor ion scans that occur as horizonal lines. Product ion scans (vertical lines on the plot) can be extracted from the 2D domain to characterize individual compounds. Ambient ionization methods like paper spray ionization lend themselves particularly well to combination with 2D MS/MS in complex sample field analysis. Figures of merit for 2D MS/MS data recorded on modified commercial ion trap instruments and on a miniature instrument are discussed. The identification of bacteria from their 2D lipid profiles is presented along with the measurements of drugs in biofluids.

Acknowledgement

This work was supported by the Department of Homeland Security and by Teledyne Inc. through DTRA funding.

Biography - Joseph Caruso

Joe is a chemistry graduate student in the Graham Cooks lab at Purdue University. His research interests center around applying miniature mass spectrometry for use in point-of-care analysis. Before grad school, Joe earned a bachelor’s degree in environmental science from The University of Scranton. He then worked at a contract research organization in New Jersey, where he performed quality control testing on pharmaceutical products and medical devices using techniques such as LC-UV and GC-FID. The combination of industry and academic experience has shaped his interests in analytical chemistry and continues to guide his current research in mass spectrometry.

Keywords

Tandem mass spectrometry, Bioanalytical chemistry, Ion traps, Neutral loss scan

Instrument Simulation --Why, What to Expect, What tools to use

Dr. Bob Jackson - United States - Ashwood labs
Mr. Mark Osgood - United States - Ashwood labs

Abstract

At past HEMS conferences, I have spoken about SIMION and our efforts to expand its usefulness, improving accuracy, using it to analyze fields, and applying it to the synthesis of ion optics. This year, I will address broader questions about the utility of simulations as partners in design and experiment.

Over my forty-year career designing scientific instruments, I have seen good reasons for skepticism toward simulations. Sometimes they were too crude, limited by the available software and computing hardware. While expectations were too high, they were high on both the simulators' part and the groups requesting the simulations. In this talk, I will revisit these misgivings, considering greatly improved software and hardware, and I will emphasize the necessary interplay among simulation (i.e., theory), intermediate experiments, and multiple-hypothesis testing—the very bedrock of expedient scientific progress.

Another key consideration today is the advent of powerful artificial intelligence tools. When used judiciously, AI can enable even infrequent users of simulation software to set up and run effective simulations, and to write code that once required deeper expertise.

I will also review recent developments in simulation tools—not only SIMION but also Multiphysics approaches, both commercial and open-source, including COMSOL, OpenFOAM, MEEP, and the MOOSE framework. While no single designer can master all of these, I hope to show that the combination of available tools and AI may usher in a renaissance in scientific instrument simulation and design—bringing models closer to reality and fostering a community of simulation practitioners more tightly integrated with instrument designers.

Finally, I will discuss the use of simple Git commands not only for revision control but also for results documentation, highlighting the workflow I have implemented in SIMION as an example. I look forward to stimulating discussion both during the talk and throughout the conference.

Biography - Bob Jackson

Bob Jackson has a BS in engineering Physics and a master's and Ph.D in Physics. He designed scientific instruments as an undergraduate and graduate student, He was a postdoctoral fellow at the Laboratory for Surface Science and Technology at the University of Maine NSF MRI grant to develop a HREELS Tof. He previously worked as an Electrical Engineer for a high-power RF transmitter company. His career has involve 4 startup scientific instrument companies and work for an Ion Mobility manufacturer.

Keywords

Scientific Instruments, Simulation, Design

Novel ship-based and submersible Membrane Inlet-Photo-Ionization Mass Spectrometer (MI-PIMS) for on-line detection of fuel spills, environmental contaminants and TNT in sea water

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Dr. Detlef Schulz-Bull - Germany - University of Rostock
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Dr. S. Ehlert - Germany - University of Rostock
Mr. Norbert Graf - Germany - InnoLas Laser GmbH
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Dr. E. Achterberg - Germany - Geomar
Dr. J. Passig - Germany - University of Rostock

Abstract

The trace analysis of anthropogenic pollutants in seawater, such as Polycyclic Aromatic Hydrocarbons (PAH) from oil spills and TNT from dumped ammunition, is crucial in marine sciences. After the World Wars, large quantities of ammunition were dumped in European coastal waters, posing a threat to marine ecosystems. Continuous monitoring is necessary. A new online analysis method combines direct water sampling via a membrane inlet with a mobile Photoionization Mass Spectrometer (MI-PIMS). The system samples seawater into a membrane extraction unit, where organic contaminants penetrate a PDMS membrane and are transported to a TOFMS. Laser pulses ionize target molecules using Resonance-Enhanced Multiphoton Ionization (REMPI), enabling real-time measurements of pollutants at ng/L levels.

The mobile MI-PIMS system was initially tested in the Warnow Estuary in Rostock, Germany, and showed high sensitivity in detecting PAH in sea water. This allows the detection of e.g., oil spills or other pollution sources. The approach was also used to detect PAH and other aromatic xenobiotics in process water from marine sulfur scrubbers, with pollutant transfer highly dependent on operating conditions. For explosive detection at ammunition dump sites, TNT and other explosives need to be detected. The target molecules penetrate the PDMS membrane and are guided via a capillary in the MS system. 226 nm Nd:YAG-OPO-laser pulses or 213 nm laser pulses (quintupled Nd:YAG) are inducing a photolytic formation of NO_2 from any nitroorganic explosive. The NO_2 molecule subsequently undergoes instantaneous predissociation, forming nitrous oxide molecules (NO) which are efficiently ionized by the same laser pulse in a 1+1-REMPI process. The NO^+ signal serves as sensitive markers for explosives.

A shipborne MI-PIMS system was developed. The system for on-line testing of sea water can be operated onboard ships in a ship deck-based container. On a research cruise with the German Research Vessel “Littorina” bottom water from ammunition dump sites in the Baltic Sea was tested. The bottom water was pumped up by a submersible probe or a small remotely operated underwater vehicle (ROV). Explosives (TNT) were successfully detected by MI-PIMS at ppb concentrations, indicating that the shells are already disintegrating.

Finally, a submersible, underwater MI-PIMS system was developed to test for PAH from oil spills and TNT traces at ammunition dump sites. The MI-PIMS system, consisting of a pressure resistant

membrane inlet, a compact reflectron TOF mass spectrometer and a fully tunable Nd:YAG-OPO laser system, was setup in an aluminums pressure housing (max. depths: 100m). The submersible MI-PIMS system is battery powered. For underwater operation it is mounted on a large ROV unit. Data communication is running via the surface connection line of the ROV. A first test of the submersible MI-PIMS/ROV system was conducted on a Baltic Sea research cruise with the German Research Vessel “Alkor”. The system was operable and able to detect trace of PAH in sea water.

Within the outlook, future development perspectives of the MI-PIMS approach are discussed.

Biography - R. Zimmermann

1995 Graduation (Dr. rer. nat.), TU Munich/Weihenstephan, 1999 Research sojourn University of Antwerp, Belgium, 2001 Professorship in analytical chemistry (C3), University of Augsburg; division manager at bifa-Umweltinstitut in Augsburg and team leader GSF (at the research centre), 2001 state doctorate (environmental chemistry and analysis), TU Munich/Weihenstephan, since 2008 Chair in analytical chemistry (W3) and head of the Joint Mass Spectrometry Centre of the University of Rostock and the Helmholtz Zentrum München, since 2022 Head of Department Life, Light & Matter (LLM)

Keywords

Underwater mass spectrometer, Photoionization, Membrane inlet, TOF, TNT, PAH

Simultaneous MIMS and UV/VIS absorption for chemical reaction kinetic studies exemplified by disinfection byproduct formation from environmental contaminants

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Ms. Ana Katharina de Arce Stöver - Denmark - University of southern Denmark
Ms. Lise Lotte Jepsen - Denmark - University of Southern Denmark

Abstract

MIMS is a well-known method for online monitoring of volatile organic compounds and is highly suitable for online monitoring of volatile organic disinfection byproducts (DBPs) formed when water is disinfected, but it cannot analyze the typical precursor compounds (pesticides, pharmaceuticals etc.) to DBP formation. This problem can be overcome by simultaneous UV/VIS absorbance monitoring of the non-MIMS detectable precursor compounds simultaneous to MIMS monitoring of the formed volatile DBPs. In practice we use an experimental laboratory reactor (ELR) fully integrated with a membrane inlet mass spectrometer (MIMS) and a handheld UV/VIS spectrophotometer. This makes it possible to simulate the reactions that occur at waterworks when drinking water is disinfected.

As examples of reactions to simulate chlorination of contaminated water, we used some of the most common non-MIMS detectable water pollutants, acetaminophen (a pain reliever), caffeine (a lifestyle drug), and difenoconazole (a common herbicide). Acetaminophen is an example of a precursor that creates toxic short-lived intermediates (benzoquinones) that can be detected by both MIMS and UV absorption, caffeine is an example of a precursor that forms a wide range of highly toxic DBPs, and difenoconazole is an example of a precursor that barely responds to chlorination.

Some of the advantages achieved using the combined online MIMS – UV/VIS monitoring are:

- Knowledge about the quantitative fate of the non-MIMS detectable precursors to be used for understanding of mass balances.
- Independent UV/VIS verification of the identity of short-lived UV/VIS absorbing degradation intermediates.
- In connection with water chlorination, it often becomes possible to determine the amount of free chlorine, that is the amount of chlorine left for reaction with the DBP precursors after reaction with easy oxidizable constituents in the raw water investigated.

The benefits of simultaneous use of MIMS for monitoring of volatile organic compounds and UV/VIS absorbance for monitoring of non-MIMS but UV/VIS absorbing compounds can easily be transferred from laboratory studies using an ELR to field applications. This simply needs a MIMS with a flow-through membrane inlet where the aqueous sample passes through a small cylindrical cuvette before entering the thermostatically controlled membrane inlet.

Biography - Frants Lauritsen

Dr. Frants Roager Lauritsen, M.Sc., Ph.D., Dr. Scient. is professor at the Department of Physics, Chemistry and Pharmacy, University of Southern Denmark (SDU), and owner of the consultancy company MIMS Systems with expertise in design and implementation of mass spectrometers for on-site, on-line monitoring of chemical and biological processes. His recent work focuses upon disinfection byproduct formation in connection with water remediation.

Keywords

Combined MIMS and UV/VIS, Chemical reaction kinetics, Disinfection byproducts, Water contaminants

SPion®: Flexible Ion Guide for Mass Spectrometry

Dr. Mazdak Taghioskoui - United States - Trace Matters

Abstract

When ions are produced far from a mass spectrometer, efficiently transferring them to the mass analyzer becomes challenging. In this presentation, I will introduce a novel technology called SPion®, a flexible ion guide based on the stacked-ring principle. SPion® enables efficient ion transport over relatively long distances, even when curved or flexed.

This flexible ion-guiding concept fundamentally changes the architecture of mass spectrometry instrumentation by removing the constraint of sample location. It allows for sample-centric analysis, where the mass spectrometer can extend to the sample, rather than bringing the sample to the mass spectrometer. This breakthrough fills a crucial gap in ambient ionization mass spectrometry and facilitates automation for high-sensitivity applications.

I will present both theoretical analysis and experimentally validated proof-of-principle demonstrations. The results show that SPion® efficiently transfers ions in both positive and negative modes, from 20 Da to several kDa. Notably, no solvent cluster ions are present in spectra obtained via electrospray ionization, and ion transfer with SPion® does not cause fragmentation. Additionally, bending or moving SPion® has no impact on ion transfer, although there is a slight drop in signal intensity compared to the original interface.

SPion® paves the way for the development of next-generation, sample-centric, high-performance peripheral technologies for mass spectrometry, including streamlined sample preparation platforms. I will also discuss some exemplary implementations of SPion®.

Biography - Mazdak Taghioskoui

Mazdak Taghioskoui is the CEO and founder of Trace Matters, with deep expertise in mass spectrometry instrumentation, particularly in platform development. He has received multiple awards for his research on miniaturized plasma sources and ambient mass spectrometry. Mazdak has led or co-led several NASA-funded R&D projects, including PICASSO and DALI, and was a 2020 winner of NASA's Science Mission Directorate Entrepreneurs Challenge for his invention of SPion®. He holds over 10 patents in mass spectrometry.

Keywords

Flexible ion guide, Ion transfer, Lossless ion transfer

Design and Performance of a Person-portable Two-dimensional Tandem Mass Spectrometer for Machine-Learning Enhanced Identification of Threats

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Mrs. Megan Guetzloff - United States - Teledyne FLIR Detection
Mr. Andy Eller - United States - Teledyne FLIR Detection
Dr. Conner Harper - United States - Teledyne FLIR Detection
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Mr. Brandon Reese - United States - Teledyne FLIR Detection
Mr. Brent Rardin - United States - Teledyne FLIR Detection
Dr. Anna Leech - United States - Teledyne FLIR Detection
Dr. Mitch Wells - United States - Teledyne FLIR Detection

Abstract

There is an urgent need for high sensitivity chemical detectors for untargeted threat detection. The proliferation of novel, cheap synthetic drugs of high toxicity has made clear that current detection solutions are insufficient when new chemical variants, often of higher toxicity than the original threat molecule, can be created easily and at low cost and then distributed worldwide. Fentanyls and nitazenes are two classes of synthetic opioid narcotics that have proliferated over the last decade, causing tens of thousands of overdose deaths every year since 2017 and showing little sign of abating despite intensified public health efforts and greater attention from law enforcement. Other chemical threats such as chemical warfare agents continue to see sporadic usage against civilian populations. A prominent 21st century example was the use of sarin gas in an August 2013 attack in Ghauta, Syria, killing more than 1,000 people and injuring thousands more. These instances highlight the need not only for highly sensitive, selective, and broadly applicable chemical detectors, but also the desire for more advanced software and algorithms so that existing tools are more adaptable to existing and emerging threats.

Current fieldable and man-portable mass spectrometers, both GC-MS and direct sampling MS (DSMS) systems, rely on comparison of experimental data acquired in the field to libraries of spectra onboard the instrument via cosine similarity scoring or similar ‘dot product’ algorithms.

While accurate, reliable, and computationally inexpensive (allowing the process to be run onboard the instrument in real time), this ‘gold standard’ approach fails to identify or even classify near-neighbor variants of molecules in the library, although hybrids of cosine similarity scoring can partially address this issue. Moreover, the onboard libraries become out-of-date quickly as new chemical threats emerge, and so the libraries must be updated periodically, allowing nefarious actors to stay ‘ahead of the curve’ by continually introducing novel threat analogs that evade existing libraries. For systems in the field, regularly updating the target libraries is often impractical or impossible (e.g. for systems that are deployed on the battlefield).

Teledyne FLIR has developed a person-portable (~33 lb) direct sampling mass spectrometer with novel two-dimensional tandem mass spectrometry (2D MS/MS) capabilities. 2D MS/MS is an untargeted analysis technique that yields rich mass spectra consisting of three dimensions of information (precursor m/z, fragment m/z, and abundance). When 2D MS/MS as an untargeted survey scan is combined with data-dependent acquisition (which we refer to as ‘intelligent’ DDA, or iDDA), the MS achieves low false positives compared to the traditional DDA approach while more intelligently acquiring MS/MS spectra. The system is further enhanced with library-less chemical identification and/or classification capabilities through novel machine learning algorithms. This presentation will highlight the design and capabilities of the MS, the novel algorithmic approaches being applied to the 2D data to achieve library-less identification of threats, and the vision for the future of the 2D MS/MS platform.

Biography - Dalton Snyder

Dalton Snyder is currently the Research & Development Manager for the Teledyne FLIR West Lafayette (IN) site, driving the development of compact, person-portable mass spectrometers for CBRNE threat detection. Prior to his tenure at Teledyne FLIR he obtained his PhD from Graham Cooks' lab at Purdue University, where he specialized in ion trap miniaturization and novel scanning methodology. He then was a postdoctoral research associate in Vicki Wysocki's laboratory focusing on instrumentation development for native mass spectrometry, culminating in the first commercialization of a surface-induced dissociation cell.

Keywords

Mass spectrometry, Miniature mass spectrometer, Portable mass spectrometer, 2D MS/MS, Machine learning, Ambient ionization

Integration of the Submersible Under-Ice Mass Spectrometer (SUIMS) with the Icefin ROV for Dissolved Gas Measurements at the Grounding Zone of a Marine-Terminating Glacier

Mr. Jorge Coppin-Massanet - United States - Cornell University
Dr. Britney Schmidt - United States - Cornell University
Dr. Peter Girguis - United States - Harvard University
Mr. Matthew Meister - United States - Cornell University
Dr. Peter Washam - United States - Cornell University
Dr. Frances Bryson - United States - Cornell University
Mr. Daniel Lein - United States - Cornell University
Ms. Veronica Hegelein - United States - Cornell University
Dr. Paul Tanghe - United States - Cornell University

Abstract

The grounding zones of marine-terminating glaciers represent one of the most dynamic and inaccessible interfaces in the cryosphere, where subglacial freshwater mixes with ocean water beneath thick ice cover. Understanding the fluxes and biogeochemical transformations that occur in these environments is critical for constraining meltwater contributions to ocean circulation, carbon cycling, and ice sheet stability. However, direct observations of dissolved gases—key tracers of subglacial hydrology and microbial activity—remain virtually nonexistent in these regions due to extreme access limitations.

To address this gap, we have developed and deployed the Submersible Under-Ice Mass Spectrometer (SUIMS), a compact in-situ membrane inlet quadrupole mass spectrometer designed for harsh polar environments. SUIMS is currently being prepared for integration into the forward payload bay of Icefin, a remotely operated vehicle (ROV) developed for glacial and under-ice exploration. Once integrated, SUIMS will enable real-time, co-located measurements of dissolved gases alongside Icefin's suite of environmental sensors, including conductivity-temperature-depth (CTD), dissolved oxygen (DO), and acoustic Doppler current profiling (ADCP).

Field tests were conducted at marine-terminating glaciers in Northwest Greenland, where SUIMS operated as a standalone unit beneath seasonal sea ice. Future deployments will use Icefin's mobility and navigational capabilities to generate high-resolution, spatially resolved maps of grounding zone discharge plumes—revealing how gas distributions evolve with flow, mixing, and subglacial source variability.

This work lays the foundation for long-duration chemical sensing in extreme under-ice environments, with applications to both Earth system science and planetary exploration.

Biography - Jorge Coppin-Massanet

Jorge Coppin-Massanet is a Ph.D. student in Geological Sciences and Astronomy at Cornell University, where he develops and deploys scientific instrumentation for harsh and remote environments. His work bridges glaciology, oceanography, and planetary science, with a focus on sensor integration, field-deployable platforms, and in-situ chemical measurements beneath ice. He has contributed to under-ice robotics efforts in polar regions and is actively involved in advancing instrumentation for subglacial and grounding zone research.

Keywords

Polar Oceanography, Cyrospere-ocean interface, Robotic exploration, Membrane-inlet mass spec

A New Aerosol Threat Detector

Mr. Gottfried Kibelka - United States - Detect-ION
Mr. Dustin McRae - United States - Detect-ION
Dr. Bob Schweitzer - United States - Detect-ION
Mr. Jeff Strickrott - United States - Detect-ION
Dr. Greg Vasquez - United States - Detect-ION
Dr. Ashish Chaudhary - United States - Detect-ION

Abstract

Non-volatile chemical compounds can persist in the atmosphere as aerosols ranging in size from nanometers (nm) to micrometers (µm), posing significant risks during acts of terrorism, industrial accidents, and environmental disasters. Real-time, in-situ detection of such airborne threats is critical for timely response and mitigation. Detect-ION (DI) is developing **SPECTRAL**, a compact, low-SWaP (Size, Weight, and Power) platform designed to collect, separate, and identify aerosolized chemical agents across a broad size range. The system integrates three novel subsystems: a Miniature Aerosol Collector (MAC), a low-thermal-mass gas chromatograph (LTM-GC), and a chip-scale mass spectrometer (µMS), leveraging prior IARPA-supported technologies.

The MAC utilizes DI's patent-pending Glass Array Collector (GLAC) design to enable efficient aerosol impaction, high surface area capture, and rapid desorption for sharp GC injections. The LTM-GC offers performance comparable to traditional ovens while operating in a compact form factor. DI's inline GC split technology enables increased sample throughput to the µMS without sacrificing separation quality. The µMS employs a high-density microfabricated ion trap array and low-power electronics to deliver ppb-level sensitivity across 40–210 m/z, with a resolution of 1–2 amu and power consumption under 3 W. The system produces NIST-compatible electron impact (EI) mass spectra, supporting rapid identification via existing spectral libraries. Prior demonstrations across >200 volatile and semi-volatile compounds validate the µMS performance.

Conflict of Interest Disclosure

This work was funded by IARPA.

Biography - Gottfried Kibelka

Gottfried Kibelka holds a master's degree in chemistry from the University of Hamburg, Germany. His passion for mobile mass spectrometers started in 1988 when he developed field methods for Bruker's pioneering MM1 system. After developing an underwater mass spectrometer for the German Coast Guard. He joined Tim Short's group, continuing his work on underwater mass spectrometry. He continued developing portable mass spectrometers throughout his career and serves now as a Senior Instrumentation Scientist at Detect-Ion, in Tampa, Florida, where he contributes to the development of next-generation mass spectrometry solutions for healthcare and environmental applications.

Keywords

Ion trap array, Miniature mass spectrometer

Multimodal Ionization Strategies for Broad-Spectrum Threat Detection with a Miniature Field Mass Spectrometer

Dr. Nathan Grimes - United States - BaySpec

Abstract

Field teams need one instrument that can ionize everything from high-proton-affinity nerve-agent simulants to low-affinity petrochemicals. We have pursued two complementary strategies on the 22 kg Continuity portable linear ion-trap: (1) an atmospheric multimodal source that merges dielectric-barrier discharge ionization (DBDI), atmospheric-pressure chemical ionization (APCI), and atmospheric-pressure photoionization (APPI); and (2) a new configuration that retains DBDI and APCI in air while relocating the deuterium lamp behind the inlet orifice to enable vacuum ultraviolet photoionization (PI) inside the first vacuum stage.

For the atmospheric design, a patented coaxial manifold couples the DBDI plasma with an APCI corona needle and directs a 10.78 eV D_2 lamp into the same reaction volume. Bench testing with permeation-tube vapors showed mode-specific advantages: 2-butanone responded best in pure APCI, toluene radical cations dominated in APPI and DBDI, and dimethyl methylphosphonate gained an additional threefold in signal intensity when all three modes were active. Operating APPI and APCI concurrently raised total ion current for every analyte studied, confirming the predicted proton-transfer and photoionization synergy.

The vacuum PI variant addresses species whose proton affinities lie below that of water yet whose ionization energies fall under 10.78 eV, for example benzene and chlorinated benzenes. A 25 mm chamber extension positions the lamp at 7 torr, upstream of the ion funnel. Three low-profile DC lenses steer ions through the new region without additional RF, an arrangement validated in SIMION and confirmed experimentally.

We are actively comparing the atmospheric multimodal source with the vacuum-PI version to determine which excels at different target classes. By combining the DBDI, APCI, and photon-based ionization in a single adaptable front end, this approach expands chemical coverage and accelerates field detection capabilities without compromising portability.

Biography - Nathan Grimes

Nathan Grimes, Ph.D. is an Instrumentation and Application Scientist specializing in miniature linear ion trap mass spectrometry. He earned his Ph.D. in Analytical Chemistry with a focus on portable MS systems, instrumentation/ionization development, and differential ion mobility. His work spans electrical, mechanical, and software integration for field-deployable systems, as well as method development for detecting trace vapors, aerosols, and complex biological or environmental samples. Dr. Grimes has authored technical reports and proposals for defense and environmental applications, and has field experience in government and military collaborative projects.

Keywords

Portability, Photoionization, Multimodal, Corona

Vertical transport of biogenic CO2, O2 and �O2/Ar in eddies and at fronts is revealed by submersible mass spectrometer

Prof. Brice Loose - United States - URI Graduate School of Oceanography
Prof. Ilker Fer - Norway - University of Bergen
Dr. Enric Pallás Sanz - Mexico - CENTRO DE INVESTIGACIÓN CIENTÍFICA Y DE EDUCACIÓN SUPERIOR DE ENSENADA
Dr. Tim Short - United States - Unaffiliated
Dr. Strawn Toler - United States - University of South Florida

Abstract

Eddy dynamics are recognized as important sources of vertical mixing and transport throughout much of the ocean, including in subtropical gyres. Here, we use high-resolution biogeochemical profiles from a vertically towed submersible wet-inlet mass spectrometer (SWIMS) to estimate how eddies alter the surface ocean distribution of $[CO_2]$, $[O_2]$, and the DO_2/Ar ratio; the last as a tracer of Net Community Productivity. The eddy surveys found net heterotrophy in late winter ($\Delta O2/Ar = -11.7\%$) and in mid-summer ($\Delta O2/Ar = -8\%$), although photosynthesis below the mixed-layer in the subsurface chlorophyll maximum is responsible for significant autotrophy in summer. All three cyclonic eddies (CEs) we surveyed brought up cold water that resulted in more heterotrophic anomalies - higher in CO_2, lower O_2, lower DO_2/Ar than the transect average. By comparison, the three anticyclonic eddies (ACEs) showed positive temperature anomalies and greater autotrophy than the transect averages. We used a two-dimensional quasi-geostrophic form of the omega equation to determine ageostrophic vertical velocities up to +/- 4 meters per day. Strong vertical velocities were coincident with perturbations in CO_2, O2, and CDOM fluorescence, yielding large biogeochemical fluxes at eddy edges and along the North Wall of the Gulf Stream. These studies show how fast-response in-situ mass spectrometry can reveal eddy processes that impact export production in the surface ocean.

Biography - Brice Loose

Brice Loose is Associate Professor at URI Graduate School of Oceanography studying marine biogeochemical and freshwater cycles in the polar oceans.

Keywords

Mesoscale ocean processes, Submersible mass spectrometer, Sargasso Sea

Development of the Dragonfly Mass Spectrometer (DraMS) for Titan

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Dr. William Brinckerhoff - United States - NASA Goddard Space Flight Center
Dr. Andrej Grubisic - United States - NASA Goddard Space Flight Center
Dr. Jacob Graham - United States - NASA Goddard Space Flight Center
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Dr. M. Joseph Pasterski - United States - CRESST II, NASA Goddard Spaceflight Center
Dr. Luoth Chou - United States - NASA Goddard Space Flight Center
Dr. Jennifer Stern - United States - NASA Goddard Space Flight Center
Dr. Arnaud Buch - France - LPGM, CentraleSupélec
Prof. Cyril Szopa - France - LATMOS
Dr. Caroline Freissinet - France - LATMOS

Abstract

Titan's abundant complex carbon-rich chemistry, interior ocean, and past presence of liquid water on the surface make it an ideal destination to study prebiotic chemical processes and habitability of an extraterrestrial environment. NASA's *Dragonfly* New Frontiers mission is a rotorcraft lander designed to perform wide-ranging *in situ* exploration on this moon of Saturn by flying to different geologic settings 10s of km apart. Multidisciplinary science measurements at each landing site will reveal the compositions of the solid materials on Titan's surface, which are still essentially unknown.

Two primary science goals of the *Dragonfly* mission are to identify chemical components and processes at work that may produce biologically relevant compounds, and to search for potential molecular biosignatures. These objectives are addressed by the *Dragonfly* Mass Spectrometer (DraMS), which performs molecular analysis on surface samples that are acquired and delivered by the Drill for Acquisition of Complex Organics (DrACO).

DraMS is a linear ion trap mass spectrometer, most closely related to the Mars Organic Molecule Analyzer (MOMA) [8], part of the ExoMars *Rosalind Franklin* Rover set to launch in the late 2020’s. For solid sample analysis, DraMS features two modes: Laser Desorption Mass Spectrometry (LDMS) for the broad compositional survey of surface materials including refractory organics, and Gas Chromatography Mass Spectrometry (GCMS) for the separation and identification of key prebiotic molecules and measurement of enantiomeric excesses (if present). LDMS mode allows for structural disambiguation of surface molecules using ion isolation and tandem mass spectrometry (MS/MS). GCMS mode uses pyrolysis or derivatization to volatilize, separate, and identify molecules of interest using electron impact ionization mass spectrometry. Much of the gas processing system (valves, pyrolysis oven, etc.) and electronics are also inherited from the Sample Analysis at Mars (SAM) instrument onboard *Curiosity.*

The DraMS instrument completed Critical Design Review (CDR) in February, 2025, followed by *Dragonfly* Mission CDR in April 2025. DraMS is now beginning the fabrication, assembly, and integration of the flight model. Much of the novel development effort has focused on areas in which the unique aspects of the *Dragonfly* mission differed from the heritage investigations. These differences range from those imposed by the Titan environment (e.g., atmospheric pressure, temperature), those imposed by the spacecraft (e.g., rotorcraft vibration environment), and those related to the Dragonfly science investigation (e.g., abundant organics, ice bedrock).

Here we will present the design and current status of the DraMS investigation and instrument development. We will focus on the science goals of the DraMS instrument and how the design is tailored to meet these goals.

Biography - Desmond Kaplan

Desmond Kaplan earned his B.S. in Chemistry from Towson University (2001) and Ph.D. in Analytical Chemistry from the University of North Carolina at Chapel Hill. He spent over a decade in R&D at a mass spectrometry company, advancing ion trap isolation, quadrupole hybrid analyzers, trapped ion mobility spectrometry, ion-ion reaction cell chemistry, and ruggedized nano-ESI triple quadrupoles. In 2017, he joined NASA Goddard's Planetary Environments Laboratory. His research centers on miniature linear ion trap mass spectrometers for spaceflight and field use. He contributes to the **MOMA and DraMS** flight instrument teams as well as several other projects at NASA.

Keywords

Ion Trap, Spaceflight, NASA, Titan

Standoff Laser Ablation Mass Analyzer (LAMA) for Lunar Surface Analysis

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Dr. Jacob Graham - United States - NASA Goddard Space Flight Center
Dr. Jane Lee - United States - NASA Goddard Space Flight Center
Dr. William Brinckerhoff - United States - NASA Goddard Space Flight Center

Abstract

Lunar exploration is central to addressing key questions about the origin and evolution of the Solar System while supporting the development of sustainable human presence beyond Earth. Future missions will require rapid, high-resolution chemical and isotopic analyses of diverse lunar materials *in situ*, at fine spatial scales, and with minimal sample preparation. The Laser Ablation Mass Analyzer (LAMA) is a novel instrument designed to meet this need by combining the efficiency of pulsed laser ablation sampling with the sensitivity and accuracy of time-of-flight mass spectrometry (TOF-MS) for operation in the lunar vacuum. LAMA integrates a Q-switched Nd:YAG laser (1064 nm) with a heritage TOF-MS design derived from Phobos-Grunt and Luna Resurs missions and introduces a unique standoff analysis mode that enables compositional measurements over adjustable target ranges from 5 cm to more than 30 cm. This approach, achieved through dynamically tunable ion optics employing shape-changing lenses made of optical fluids and polymer membranes, eliminates the need for bulky mechanical components, allowing for a compact, few-kilogram payload with low power demands ideally suited for robotic landers, rovers, or astronaut-deployed platforms. Laboratory testing with lunar analog materials demonstrates ppmw detection limits for many rock-forming and trace elements, semi-quantitative determination of elemental ratios within ±10% relative standard deviation, and fine-scale (micron to millimeter) resolution suitable for heterogeneous samples. High-intensity laser operation enables correlated detection of H^+ and O^+ ions for water ice prospecting, supporting both scientific investigations and resource prospecting for human exploration. Furthermore, LAMA can operate semi-autonomously to locate and characterize high-priority phases across an exploration area and can be used within astronaut habitats for detailed follow-up studies of collected samples, complementing other instruments. By enabling chemical, isotopic, and mineralogical analyses directly on the lunar surface without sample handling, LAMA significantly advances the ability to provide ground truth for orbital observations and identify resource-rich regions critical for sustained exploration. This instrument represents a transformative step in standoff mass spectrometry for planetary missions, offering a much-needed capability for efficient, high-resolution, and non-destructive surface analyses that directly address priority lunar science and human exploration objectives of the coming decade and beyond.

Biography - Xiang Li

Xiang Li received his Ph.D. in Physical Chemistry from the Johns Hopkins University in 2009. He is a mass spectrometry scientist at NASA Goddard Space Flight Center. His research focuses on the detection of trace element and astrobiologically relevant organic molecules in planetary systems, such as Mars, Europa and Titan. He is especially interested in the instrument development of time-of-flight and ion trap mass spectrometers with various ionization and ion gating techniques.

Keywords

LAMA, Standoff, Lunar surface

Under Water Coded Aperture Miniature Mass Spectrometer for Measurements of Methane Content in the Ocean

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Abstract

Methane hydrates, solid complexes of water and methane, naturally occur in permafrost sediments and beneath the ocean floor[1]. Remarkably, under standard temperature and pressure, dissociation of one cubic meter of methane hydrate can yield up to 164 cubic meters of methane gas[2]. These hydrates remain stable within a narrow range of pressure and temperature conditions[3]. However, global warming can disrupt this stability, potentially leading to a catastrophic feedback loop between climate change and methane release from methane hydrate reservoirs. The exact pathways of methane release and its metabolism in the ocean water column remain unclear[1, 3], as *in situ* methane content measurements are still challenging. Currently, the most common method involves collecting seawater samples in canisters for laboratory analysis [4, 5], which is expensive, introduces potential errors, and does not provide the real-time data that can help guide sampling strategies. To address these challenges, we are developing an underwater coded aperture miniature mass spectrometer[6] for *in situ* methane measurements in the ocean water column. This instrument will not only be applicable to methane released from methane hydrates but also to other oceanographic and biogeochemical research questions. Our mass spectrometer integrates three key technologies: a

cycloidal mass analyzer, a capacitive transimpedance array detector, and a spatially coded aperture[6]. The gas content in the water will be sampled using a high-pressure membrane inlet[7]. The entire instrument, including control boards, pressure vessel, mechanical parts, cooling system, has been designed, simulated, and fabricated. We will present the design and fabrication of the instrument, including details of the control board[8] and preliminary calibration curves of low concentrations of methane/air in water.

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Biography - Rafael Bento Serpa

Rafael Bento Serpa is a Research Scientist at Duke University. He holds a Ph.D. in Physics, along with bachelor's degrees in Physics and Electronic Engineering. His scientific career began in the field of materials science, where he focused on electrochemical systems with applications in photocatalysis and organometallic solar cells. Since 2019, he has been working at Duke University on the development and application of mass spectrometry instrumentation for isotopic ratio analysis and the quantification of dissolved gases in oceanic environments.

Keywords

Under water MS, Methane measurement in ocean water, Depth profile of methane concentration, Cycloidal mass analyzer

Extraterrestrial Molecular Indicators of Life Investigation (EMILI): Development of Flight-Like Prototype

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Abstract

Introduction: The Extraterrestrial Molecular Indicators of Life Investigation (EMILI) is an instrument concept under development for future potential astrobiology missions to Enceladus, Europa, Mars, and beyond. Alien molecular biosignatures may or may not share similarities to those of terrestrial life. In situ analyses must be prepared to detect and characterize a wide range of possible molecular species, structures, and patterns, typically with exquisite sensitivity and within a complex, unknown planetary environment. EMILI is designed to meet ambitious requirements for broad organic molecular analysis on future missions such as the conceptualized Enceladus Orbilander through chemical separation systems coupled to both optical and mass spectrometry detection. These are realized in an integrated, compact package compatible with anticipated flight environments.

Design: To detect and characterize *the broadest inventory* of organic molecules ranging over molecular weights to at least 1000 Da with varying volatilities and polarities spanning classes of potential biotic and abiotic structures, EMILI merges the complementary front-end separation techniques of liquid-based capillary electrophoresis (CE), including laser-induced fluorescence (LIF) and conductivity detection; and gas-based pyrolysis/ derivatization gas chromatography (GC), both coupled to a common highly sensitive ion trap mass spectrometer (ITMS). The Organic Capillary Electrophoresis Analysis System (OCEANS) incorporates liquid-based sample extraction and a CE-based subsystem for analysis of polar organics and inorganic salts. The Gas Analysis Processing System (GAPS) incorporates gas-based sample extraction and both GC and Evolved Gas Analysis (EGA) subsystems targeting non-polar organics, gases, and biominerals. OCEANS and GAPS both interface to an ion trap mass spectrometer (ITMS) derived and enhanced from the Mars Organic Molecule Analyzer (MOMA) and the Dragonfly Mass Spectrometer (DraMS) instruments, for sensitive molecular analysis. The EMILI ITMS also includes a novel electrospray ionization interface, a wide mass range, and tandem mass spectrometry providing complete molecular characterization capabilities.

Development: EMILI has been integrated in various breadboard configurations to demonstrate feasibility of design elements and flight-like operations with adjustable and interchangeable components and assemblies. Testing has focused on the end-to-end performance of GAPS-ITMS (GC-MS) and OCEANS-ITMS (CE-MS) within flight constraints as these interfaces are key elements of the eventual flight concept. With the successful demonstration of breadboard performance, engineering test units (ETUs) of the subsystems have been designed and are under fabrication in a flight-like size and form factor for thermal-vacuum and vibration testing. Sample interface and electronics designs are also being adapted for the integrated EMILI configuration for various mission concepts and operational scenarios.

Biography - William Brinckerhoff

William Brinckerhoff is Senior Scientist for Life Detection in the Solar System Exploration Division of NASA's Goddard Space Flight Center, involved in the development of mass spectrometers and associated technologies for planetary missions to Mars, the Moon, Titan, and other bodies.

Keywords

Ion trap mass spectrometer, Astrobiology, Spaceflight mass spectrometry, CE-MS

Underwater Mass Spectrometry Advancements for Real-time Geochemical Analysis of Deep-sea Cold Seeps

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Mr. Malte Höhn - Germany - AWI-Bremerhaven

Abstract

Offshore oil and gas reservoirs commonly release fluids to the seafloor through hydraulic fracturing, caused by hydrostatic overpressure within the reservoir. This phenomenon is evidenced by associated blow-out pockmarks, seismic piping anomalies, and deep-sea hydrocarbon cold seeps. As a result, these seeps provide a means of characterizing fluids and brines transported directly from reservoir bodies. Integrating information from these fluids with other sensing methods offers profound insights into hydrocarbon risk, leakage, maturity, source, and migration. Modern laboratory geochemical seep data offers a wealth of information, but two simple parameters stand out: measurements of readily diffused or broken-down components, which indicate the presence of "live" seep fluids, and ratiometric alkane measurements. The latter are crucial for reservoir source assessment tools like Bernard diagrams, enabling quick discrimination between biogenic and thermogenic hydrocarbons.

In situ analyzers capable of determining multiple hydrocarbons simultaneously in real-time enable cost effective, adaptive, seep sampling strategies. To effectively characterize seeps, ratiometric determinations necessitate optimized analytical accuracy and detection limits across a wide concentration range. The Underwater Mass Spectrometer (UMS) developed at Beaver Creek Analytical, LLC (BCA) has been designed and commercialized for real-time, *in situ* ratiometric dissolved gas measurements at depths up to 3000 m. This technology has been deployed at over 200 deep-sea seeps, leading to the characterization of seep hydrocarbons and their associated dissolved gas plumes.

To enable these measurements, the UMS has undergone a number of upgrades in recent years. The inlet now uses a laser cut membrane support capable of sustaining hydrostatic pressure equivalent to 3000 m water depth. The vacuum transfer line is designed to include an optional water trap, which improves detection limits by freezing water between the inlet and the analysis chamber. Detection limits have been further improved through ion source optimizations. Each component, including mass spectrometer data collection and analysis, is performed by a single microcontroller board.

Subsea valves located externally to the mass spectrometer's subsea vessel have significantly improved subsea operations, leading to numerous analytical advancements. These include:

- **Steady State Analysis**: Recirculating seawater that has already passed through the analyzer enables the sample to achieve steady state with the UMS and provides quantitative conditions.
- **External Standard Introduction**: Stored in gas-tight syringes or bags, standard seawater solutions facilitate calibrations that effectively negate the influence of ambient temperature and pressure variability.
- **Sample Collection**: Pulses of the external standards enable precise timing calibrations. Knowing system timing allows BCA's UMS to trigger the collection of target-positive discrete samples. These samples can then be analyzed in an accredited lab for complete compositional and isotopic analyses.

The BCA UMS embodies numerous analytical improvements while maintaining a focus on ruggedization and reduction in size and weight, making it uniquely suitable for field-portable applications. In addition to providing real-time geochemical data from specific fluid point sources using precisely controlled platforms (e.g., ROVs), it has successfully guided autonomous underwater deployment platforms (e.g. AUVs). Data from recent cruises, totaling over 26 weeks at sea, will be used to illustrate these advancements.

Biography - Ryan Bell

Ryan J. Bell, Ph.D., is a chemical oceanographer and engineer specializing in the design and deployment of chemical sensing systems for environmental monitoring in harsh conditions, with extensive experience in mass spectrometry, real-time data visualization, and data analysis, supported by academic teaching roles, professional appointments, patents, and numerous scientific publications. His work aids clients and partners in fulfilling adaptive sampling strategies to help make cost-effective campaign decisions. Ryan leads research, manages projects, and publishes papers on advanced instrumentation for geotechnical surveys. Survey targets have included seafloor hydrates, well-head blow-out plumes, fugitive emissions, anoxic basins, and cold-seep fields.

Keywords

Deep-sea cold seeps, Dissolved gas measurements, Ratiometric alkane measurements, Real-time geochemical analysis

Concurrent Cloud Distributed Simulation with Space Charge using SIMION

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Abstract

To design, characterize and optimize recirculating devices such as ion traps it is often necessary to simulate with a sufficiently large number of particles and with space charge effects accounted for. This is a computationally intensive task and can quickly exceed the computing resources of a single workstation. In this work we present an architecture developed that allows particle trajectory and space charge accounting to be distributed across arbitrarily scalable cloud-based computing resources. This same arbitrarily scalable architecture also enables massively paralleled exploration of operational parameter space for the purposes of device optimization. Post processing of large simulation result data sets is implemented in Jupyter notebooks taking full advantage of big data tools such as pandas data frames and various visualization frameworks such as matplotlib, seaborn and others.

Biography - Mark Osgood

Mark Osgood has over 25 years of experience in the design, construction and commercialization of mass spectrometers and analytical instrumentation. He served as a R&D physicist and project manager for TOF-MS product development at Bruker Daltonics, and was the Vice President and Director of Engineering of Excellims Corporation. In 2021 Mark Co-founded the Ashwood Labs where he serves as a principal R&D Engineer and Physicist. He holds numerous patents in the analytical field and received his BS in Physics from the University of New Hampshire.

Keywords

SIMION, Distributed computing, Simulation, Cloud, Space charge

Surface Induced Dissociation (SID) with Quadrupole Mass Filters: MS/MS without Collision Gas

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Dr. Luke J. Metzler - United States - Ardara Technologies, LP

Abstract

Surface Induced Dissociation (SID) is well recognized to provide analytical information about chemical species, via MS/MS. Compared with Collision Induced Dissociation (CID), SID promises more reproducible energy resolved breakdown curves, and access to higher energy fragmentation pathways, which can increase selectivity for MS/MS experiments.

CID generally has much better conversion efficiency of parent to progeny ions (approaching 100% in some cases involving ion traps), which in turn increases ultimate sensitivity. For the chemical species that we analyzed, we found typical SID conversion efficiency to be ~20%, not as efficient as ion traps claim, but still analytically useful.

A major disadvantage to CID for MS/MS, at least for quadrupole instruments, is the requirement for bottled pure collision gas, with its associated plumbing, regulators and flow control and pressure measurement, as well as the additional pumping required to get rid of the collision gas after you leak it into the chamber.

MS/MS using a tandem quadrupole configuration promises less ambiguous results than in an ion trap configuration due to the ion trap's potential complications of space charge and ion molecule reactions.

This work explores the analytical utility of SID for tandem quadrupole MS/MS, both in selectivity and sensitivity.

A component electrospray quadrupole mass spectrometer was configured with a 9.25mm round rod resolving quadrupole, followed by an in-line SID collision cell, followed by a collision-free RF-only rectilinear quadrupole ion guide, leading into a second 9.25 mm resolving quadrupole mass filter and electron multiplier detector.

The SID collision assembly consisted of an entrance lens, an exit lens, with a split pair of SID surfaces in between, for a total ion path length of 0.6 inches.

A novel self-assembled monolayer of 2-perfluorohexyl ethyl thiol was deposited onto a polished copper surface, and SID performance using this surface was compared to untreated polished stainless steel, with the two surfaces being mirrored halves of the center split lens pair.

The collision-free ion guide was included in these experiments to evaluate the timeline of progeny ion formation. Ions born immediately upon interacting with the surface would be expected to have an effective birth potential of the surface, whereas ions born inside the ion guide would be expected to have an effective birth potential matching the ion guide centerline potential. The final instrument does not require this ion guide.

Ion fragmentation energetics were studied for various species to better understand the advantages and trade-offs of SID versus CID for MS/MS.

Finally, we will present a proposed size and cost reduced quadrupole SID MS/MS system suitable for non-traditional installations where access to bottled gases is inconvenient.

Biography - Randall E. Pedder

Randall Pedder, Ph.D. is founder and President of Ardara Technologies L.P., a designer and manufacturer of quadrupole, TOF, and ion trap mass spectrometers and related components. Randy graduated from the University of Florida in 1992, under the guidance of Richard Yost, with a Ph.D thesis entitled “Fundamental Studies in Quadrupole Ion Trap Mass Spectrometry”. Randy has spent the last 35 years working at instrument companies doing research, product development, and collaborating with researchers worldwide, with a specific interest in providing enabling technologies for research and development of portable mass spectrometers. Past employers included Finnigan MAT, Inficon, Extrel, and Waters.

Keywords

SID, MS/MS, Quadrupole mass filters, Fundamentals