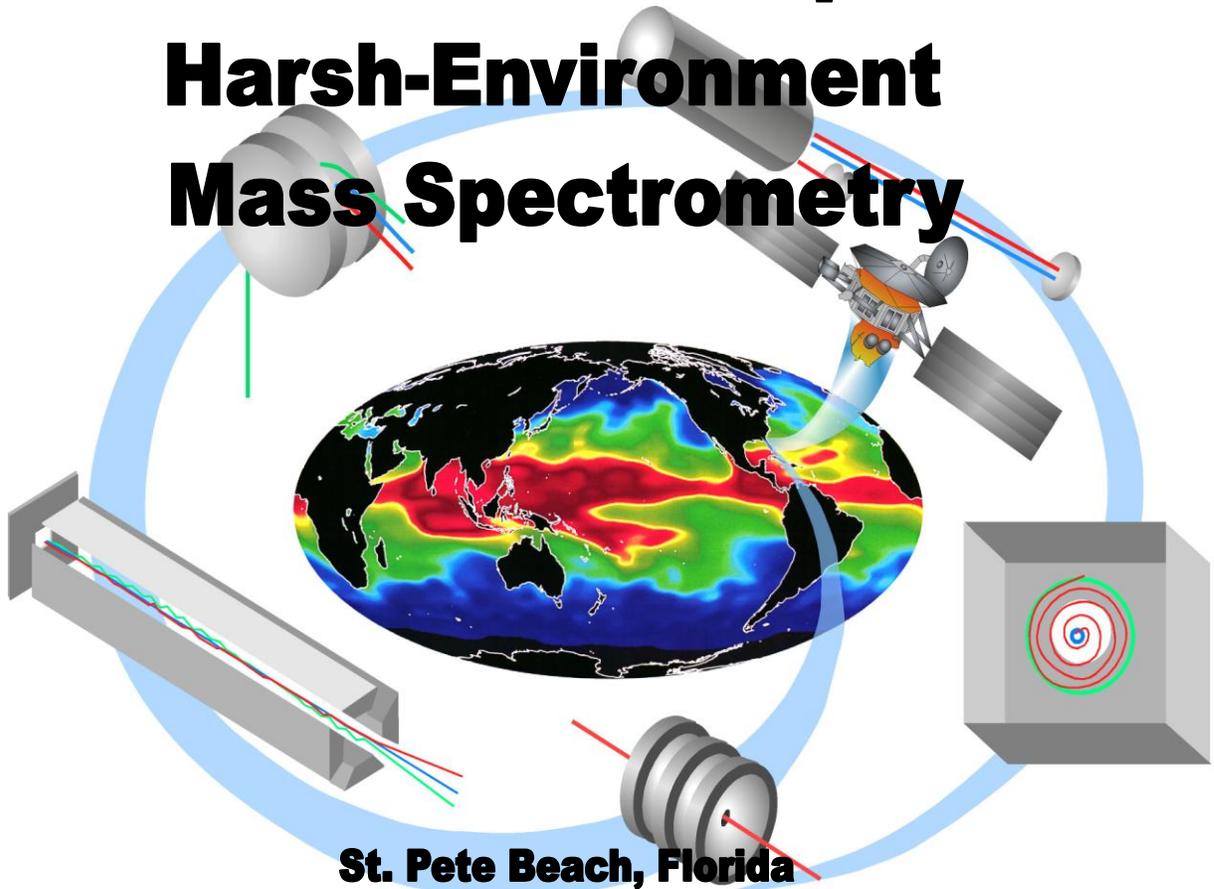


The 8th Workshop on Harsh-Environment Mass Spectrometry



**St. Pete Beach, Florida
19-22 September 2011**



WELCOME

On behalf of the Organizing Committee and HEMS Board, welcome to the 8th Workshop on Harsh Environment Mass Spectrometry (HEMS).

During this anniversary of the events on 9/11, in the wake of the Gulf Oil Spill, and recent natural disasters we are reminded of the eminent need to ruggedize and portabilize one of the most versatile and sensitive chemical sensors of our day. We are all fortunate to be part of this active community, and I appreciate all the contributions of this group to take these instruments well beyond the boundary of the lab. To places such as: battlefields, space, active volcanoes, below our seas, and often hazardous environments. This community has also led the way to novel front-end development, peripherals, and ruggedization techniques.

The 8th Workshop is a culmination of academics, government leaders, and industrial professionals brought together by a common interest to forward progress for field mass spectrometry and ruggedization. Dissemination of individual group progress will be carried out in oral and poster formats. The well needed sponsorship and vendors will offer an opportunity to interact directly with the companies and groups with market products.

The program will include time for discussion between presentations, as well as a social platform to meet and discuss projects and future directions for deployable mass spectrometry. Thank you for supporting HEMS and I look forward to the current presented research, and the discussions for future directions.

Sincerely,

Guido F. Verbeck
President HEMS
Chairman, 8th HEMS Workshop Organizing Committee

STUDENT TRAVEL AWARD WINNERS:

Josh S. Wiley, Purdue University, West Lafayette, IN
Johannes Lang, Giessen University / GSI, Germany

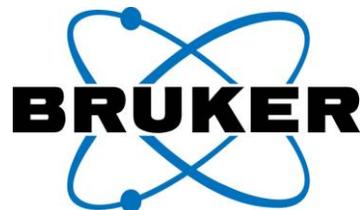
8th HEMS Workshop Organizing Committee

Guido Verbeck, *Chairman*
Ben Gardener, *Treasurer*
R. Timothy Short, *Advisor*
Strawn Toler, *Web/Materials*
Gottfried Kibelka, *Student Scholarships*
Steve Taylor, *Publications*
William Hoffmann, *Program*
Barbara Walton, *Program*

Harsh-Environment Mass Spectrometry Society Board

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Ben Gardener, *Treasurer*
Strawn Toler, *Secretary*
Directors without portfolio:
Richard Arkin
Gottfried Kibelka
R. Timothy Short
Steve Taylor
James Wylde

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History of the HEMS Workshop

The Harsh-environment Mass Spectrometry (HEMS) Workshop was created in 1999 as a means of encouraging interaction among people involved in deploying mass spectrometers outside of the typical laboratory setting. These environments are diverse, ranging from volcanoes and battlefields, to ocean depths, outer space and other rugged locales. Building mass spectrometers to withstand the rigors of such harsh and remote environments places a unique burden on engineering design and science objective planning, where operational requirements for power, size, and durability must be met while achieving the goals of the scientific mission. We hope to foster and promote interaction between scientists and engineers through the informal setting of the HEMS Workshop and thus stimulate the development of HEMS technology and applications.

Previous Workshops

1st Workshop on Harsh Environment Mass Spectrometers

February 21-23, 1999; St. Petersburg, Florida

Sponsored by the University of South Florida, Marine Science Department, Center for Ocean Technology

2nd Workshop on Harsh Environment Mass Spectrometry

March 18-21, 2001; St. Petersburg, Florida

Presented by the University of South Florida, Marine Science Department, Center for Ocean Technology

The 3rd Harsh-Environment Mass Spectrometry Workshop & The 2nd NASA/JPL Miniature vacuum Pumps Workshop

March 25-28, 2002; Pasadena, California

Presented by the Jet Propulsion Laboratory/NASA

The 4th Harsh-Environment Mass Spectrometry Workshop

October 7-10, 2003; St. Petersburg, Florida

Presented by the Center for Ocean Technology, University of South Florida College of Marine Science

The 5th Harsh-Environment Mass Spectrometry Work shop

September 20-23, 2005; Lido Beach, Sarasota, Florida

Presented by the Center for Ocean technology, University of South Florida College of Marine Science

The 6th Harsh-Environment Mass Spectrometry Workshop

September 17,20, 2007; Cocoa Beach, Florida

Presented by the ASRC Aerospace Corporation, Kennedy Space Center

The 7th Harsh-Environment Mass Spectrometry Workshop

September 21-24,2009; Santa Barbara, California

Presented by the Hamilton Sunstrand Corporation

The 8th Harsh-Environment Mass Spectrometry Workshop

September 19, 21, 2011; St. Pete Beach, Florida

Presented by the University of North Texas

For programs, proceedings, and participants please visit:

<http://www.hems-workshop.org/Archive.html>

Opening Talk: Kevin Lothridge, Chief Executive Officer – NFSTC’s principal investigator

Mr. Lothridge is an accomplished forensic scientist with 17 years of operational experience, having held positions as a forensic chemist, chief forensic chemist, and laboratory director for the Pinellas County Sheriff’s Department and the Pinellas County Forensic Laboratory. In 2006–07, he led the development of the Deployable Forensic Laboratory project for the Department of Defense. Because of his expertise, Mr. Lothridge has testified in court more than 50 times as an expert in controlled substances and fire debris analysis. He also speaks at numerous professional conferences, and he co-authored the GC-MS Guide to Ignitable Liquids.

Mr. Lothridge holds a bachelor’s degree in Forensic Science from Eastern Kentucky University and a master’s degree in Management from National-Louis University. He has served as president of the American Society of Crime Laboratory Directors (ASCLD) and as acting chief of the Investigative and Forensic division of the National Institute of Justice (NIJ). In his role as CEO of NFSTC, he provides leadership, direction and vision for the organization.

The National Forensic Science Technology Center (NFSTC)

The National Forensic Science Technology Center (NFSTC) is a 501(c)(3) not-for-profit corporation headquartered in Largo, Florida. Founded in 1995, the NFSTC provides quality forensic services including training, assessment, technology evaluation and assistance to the justice and forensic communities. NFSTC receives funding from the National Institute of Justice and other federal agencies. NFSTC founded and maintains NIJ’s Forensic Technology Center of Excellence and the National Missing and Unidentified Persons System (NamUs).

www.nfstc.org

Monday, September 19

Time	Topic	Speaker	Page #
7:00 pm	Registration		
	Meet & Greet (Light Refreshments will be available 7-9pm)		
	(See Page 13 for Floor Plans of Don CeSar)		

Tuesday, September 20

Time	Topic	Speaker	Page #
7:00	Breakfast		
8:40	Welcoming Remarks	T. Short	
9:00	Opening Talk: Traditional Tools in Non-Traditional Environments: Forensic Science in the Field	K. Lothridge	14
9:30	Underwater Cryotrap - Membrane Inlet System (CT-MIS) for Improved <i>in situ</i> Analysis of Gases by Mass Spectrometry	T. Gentz	15
10:00	Mid-Morning Break		
10:30	Underwater Membrane Introduction Mass Spectrometers: Recent Developments and Deployments	T. Short	16
11:00	Modular Quantitative Air Sampling for Field Analysis using Person-Portable GC-MS	P. Smith	17
11:30	A Suite of Sampling Aids for the In-Field SPME Collection of Analytes from Air, Particulates, and Surfaces	S.A. Lammert	18
12:00	Lunch on your own		
1:30	The Sample Analysis at Mars (SAM): Developing Analytical Tools to Search for a Habitable Environment on Mars	D. Harpold	19
2:00	Applications of Field-Mobile Purge and Trap GC/MS for Onsite Water Analysis	G. Patterson	20
2:30	Oil-in-Water Monitoring in the North Sea using Membrane Inlet Mass Spectrometry	S. Taylor	21
3:00	Magnet Portable Mass Spectrometer for Direct Control of Gases in Sea Water	A. Antonov	22
4:00	Poster Session	See Abstracts	49-53
	(Light Refreshments will be available during poster session)		
	Evening Free		

Wednesday, September 21

Time	Topic	Speaker	Page #
7:00	Breakfast		
8:15	Announcements		
8:30	Mobile High-Resolution Multiple-Reflection Time-of-Flight Mass Spectrometer for in-situ Analytics	J.Lang Student Award Winner	24
9:00	New Person Portable Gas Chromatograph for Harsh Environments – Design Criteria, and Verification Testing	J. Jones	25
9:30	Development of a Miniature Rectilinear Ion Trap Array with Independently Controlled Channels	P. Hendricks	26
10:00	Group/Photo & Mid-Morning Break		
10:30	Redesign of the VAPoR Miniaturized Pyrolysis TOFMS for Improved Sensitivity	A.E. Southard	27
11:00	Recent Advances in Portable Mass Spectrometry Systems at Kennedy Space Center	C.R. Arkin	28
11:30	Cylindrical Toroidal Ion Trap Mass Spectrometer	D. Austin	29
12:00	Lunch on your own		
1:30	Design and Use of Portable and Compact Sampling Systems for Mass Spectrometers	K. Wright	30
2:00	Design of Pocket Mass Spectrometer in a Mobile Phone Size	M. Yang	31
2:30	Mid-Afternoon Break		
3:00	A Completely Handheld Ambient Ionization Source for Mass Spectrometry Based on a Low-Temperature Plasma (LTP)	J.S. Wiley Student Award Winner	32
3:30	A Miniaturized Laser-Ablation Mass Spectrometer Designed for in-situ Measurements on Planetary Space Missions	A. Riedo	33
4:00	Autoresonant Ion Trap Mass Spectrometry (ART MS)	G.A. Brucker	34
6:30	Workshop Dinner at The Don CeSar		

Thursday, September 22

Time	Topic	Speaker	Page #
7:00	Breakfast		
8:15	Announcements		
8:30	Negative Ions for Fieldable Mass Spectrometry	W.B. Whitten	35
9:00	Mobile Mass Spectrometer in Daily Use – Experiences Made by Non-Scientific Operators	T. Ludwig	36
9:30	Utilization of Lightweight MS based Instrumentation and Small UAV Platforms for In- Situ Volcanic Plume Analysis	J.A. Diaz	37
10:00	Mid-Morning Break		
10:30	A Transportable FTICR/MS for Direct and Real- Time Analysis of VOC Contaminants in Air and Water	E.Louarn	38
11:00	Low Power Atmospheric Gas Sampling System Based on ART MS Sensor and NEG-Ion Pump System	G.A. Brucker	39
11:30	Program Survey and Closing		

The Don CeSar Beach Resort:



Opened in 1928 by Thomas Rowe, the "Pink Lady" or Don Ce-Sar, quickly became a hot spot for the rich and famous during the Jazz Age. Patrons included, Clarence Darrow, F. Scott Fitzgerald, Lou Gehrig, Franklin D. Roosevelt, and Al Capone. The New York Yankees called this place home during spring training for three years during the Great Depression. In December 1942, the hotel was reopened as a military hospital, and in 1945 it was converted again into a Veterans Administration Regional Office. Almost 30 years later, the hotel was bought by a Holiday Inn franchise owner and reopened in 1973 as The Don CeSar. It was named to the National Register of Historic Places in 1975, and has been the film site for movies (Once Upon a Time in America and Thunder in Paradise), music videos (Tom Petty and the Heartbreakers), and provided material for comedian Ron White as he talk about his stay at the Don CeSar in Blue Collar Comedy Tour: One for the Road.

The wireless network that will be available for conference use in the meeting rooms is named "SWANK" and no password is required.

St. Pete Beach, Florida

Restaurants:

<http://www.stpetebeach.com/restaurants>

- Frenchy's Seafood
- Woody's Waterfront
- PJ's Oyster Bar
- The Lobby-Downtown's Martini Bar

Attractions:

<http://www.stpetebeach.com/attractions>

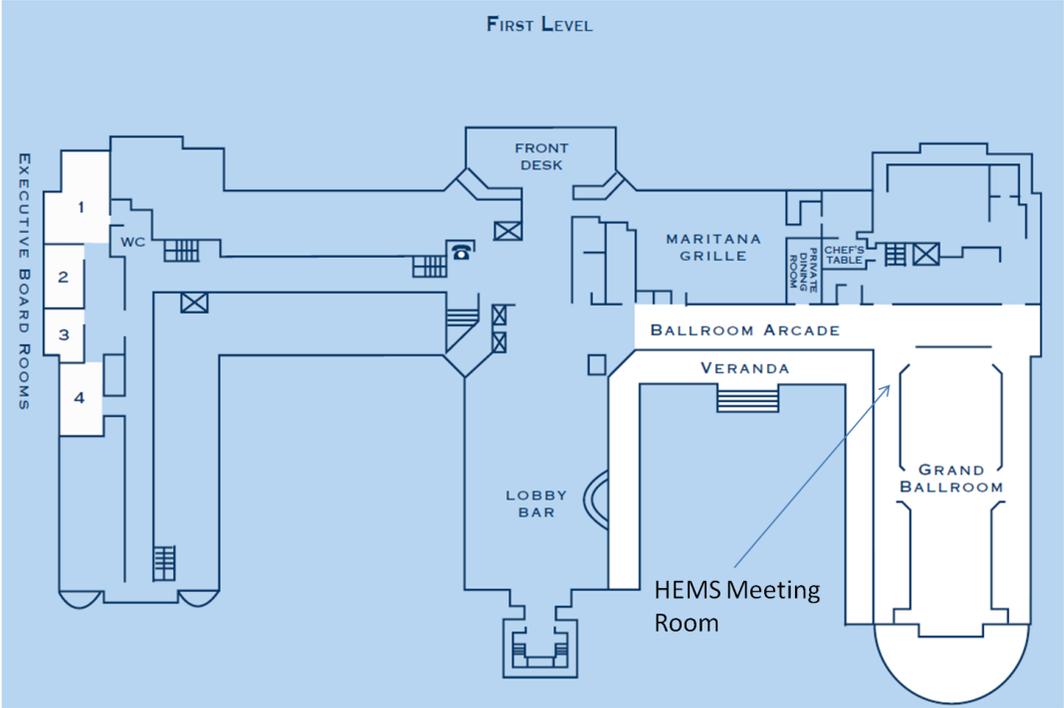
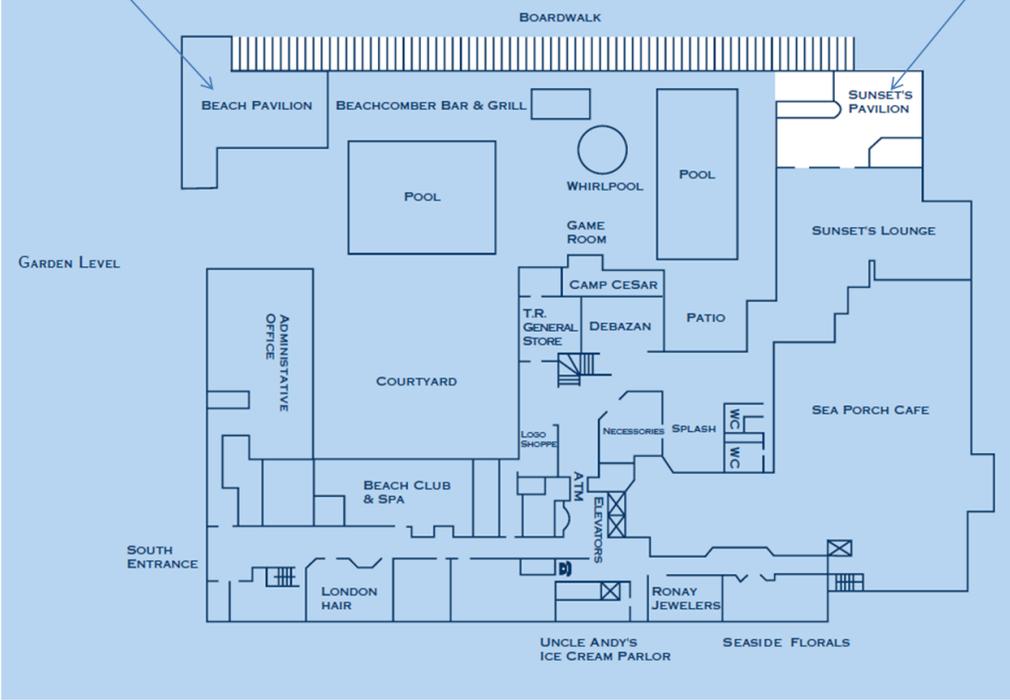
- Armed Forces Museum
- The Florida Aquarium
- Ruth Eckerd Hall



Meeting Locations in Don CeSar

Welcome Mixer
Monday, 7-9pm

HEMS Banquet
Wednesday, 7-9pm



Traditional Tools in Non-Traditional Environments: Forensic Science in the Field

K. LOTHRIDGE

The National Forensic Science Technology Center (NFSTC)

Forensic science training for soldiers in theater continues to grow in importance and timeliness, but most soldiers don't have a PhD in chemistry, never mind a background that includes scientific training. How do we take the best chemical identification tools and put them in the hands of the best warfighters to save lives and gather critical data? NFSTC regularly trains special operations soldiers to do just that by streamlining training on applied chemical detection and mass spectrometry specifically for harsh and remote environments. By providing simplified job aids and hands on practice for detection, maintenance and reach back, trained soldiers can acquire a high degree of competence in a short time. NFSTC routinely looks for and evaluates tools that can be applied in varied environments consistent results. This presentation will cover techniques used to train soldiers and other non-scientists such as law enforcement officers, and share some of the outcomes from this work.

Underwater cryotrap - membrane inlet system (CT-MIS) for improved in situ analysis of gases by mass spectrometry

T. GENTZ & M. SCHLÜTER

Alfred-Wegener-Institute for Polar and Marine Research, Bremerhaven, Germany

Membrane inlet mass spectrometer (MIMS) allows online, real time, onsite and simultaneous analysis of trace gases during investigations of terrestrial as well as aquatic environments. For applied as well as pure research investigations of gases like methane, higher hydrocarbons or CO₂ are of specific interest.

The large quantity of water vapor passing the membrane inlet downgrades the detection limit, affects the ionization efficiency, or could cause condensation of water within the sensor section. These effects can be reduced by application of cryotraps. Whereas a wide range of cryotraps are available for application in the laboratory, for field measurements or deployments of underwater mass spectrometers there seems to be still a demand for compact and robust cryotrap systems. Required features of such a system are a small size and weight as well as energy consumption below 10 Watt.

Especially for application of underwater mass spectrometers (UWMS), we designed a cryotrap system that reduces the water vapor in the analytical line significantly and build a security system to protect the sensor unit in case of membrane rupture. The in situ cryotrap is a robust system within a self-contained pressure housing and is operated at -85°C.

We present the results of the assessment of the systems, in terms of the waste heat to cope with, the efficiency to trap water vapor, as well as side effects caused by trapping gases to be analyzed. Improvements of detection limits as well as signal stability are discussed. Furthermore the design of the MIS is considered. Beside the system assessment, field results derived by the underwater cryotrap system coupled to the UWMS InSpectr200-200 are presented.

Underwater Membrane Introduction Mass Spectrometers: Recent Developments and Deployments

R.T. SHORT¹, S.K. TOLER¹, R.J. BELL¹, and R.H. BYRNE²

¹*SRI International*

²*University of South Florida*

The need for chemical monitoring and profiling in our oceans is driven by basic scientific questions as well as more pressing considerations such as the recent Deepwater Horizon oil spill. Versatile in situ analyzers are needed to locate, map, and monitor the long-term fate of chemical compounds. In situ mass spectrometers fill this need with capabilities that far exceed traditional underwater chemical sensing techniques with respect to dynamic range, and to sensitivity and selectivity to a broad range of analytes. SRI International's in situ membrane introduction mass spectrometry (MIMS) instruments can quantitatively detect volatile organic compounds in water at trace levels, while simultaneously monitoring the concentrations of all light, stable dissolved gases to a depth of 1500 meters. Recent deployments of the UMS systems in the Santa Barbara Channel and the Gulf of Mexico will be discussed. In addition, the ever-growing concerns regarding global warming and ocean acidification have led to a significant interest in developing in situ methods to characterize the oceanic carbon system. Toward this goal, we will present a novel method to simultaneously determine the partial pressure of carbon dioxide ($p\text{CO}_2$) and total dissolved inorganic carbon (DIC) in seawater using MIMS.

Modular Quantitative Air Sampling for Field Analysis using Person-Portable GC-MS

P. SMITH , S. STRATING, D. WHITE

U.S. Department of Labor – OSHA, Health Response Team; Uniformed Services University of the Health Sciences, Department of Preventive Medicine and Biometrics; Uniformed Services University of the Health Sciences, Department of Preventive Medicine and Biometrics

Thermal desorption is well suited for the introduction of analytes trapped on sorbent for quantitative analysis using gas chromatography-mass spectrometry (GC-MS). A traditional approach for thermal desorption with laboratory GC-MS analysis involves heating a packed tube containing several hundred milligrams of sorbent, and requires primary desorption flow much greater than that of carrier gas through a capillary GC column. Preconcentration on a very small volume of sorbent is thus required before the desorbed analytes may be introduced into the GC inlet to match the flow through the GC column, and heated transfer lines and bulky thermal desorption equipment are typically used. We report the use of a small diameter needle packed with sorbent as a preconcentrator to accept analytes from a traditional thermal desorption tube using a compact transfer heater separate from the analytical instrument. Controlled carrier gas flow through the needle trap that matches the GC column requirements, and simultaneous heating in the small GC injector of the person-portable GC-MS instrument used allowed quantitative analyte introduction without the need for split injection. Analytes ranging from toluene to tributyl phosphate produced a linear response from the instrument's toroidal ion trap mass spectrometric detector when about 10 to 100 ng of each was desorbed from a large sorbent tube onto the needle trap for introduction into the person-portable instrument. This corresponded to airborne concentrations in the single digit ppb range with a five minute sample time at an air sampling rate of 100 mL/minute through the large sorbent tube. A combined sampling and analysis time of 15 minutes is possible using this approach, without the need to alter the person-portable GC-MS instrument or to reduce the ability to move the instrument that would result from the use of a typical thermal desorption apparatus.

A Suite of Sampling Aids for the In-Field SPME Collection of Analytes from Air, Particulates, and Surfaces

S.A. LAMMERT¹, G.S. GROENEWOLD², J.R. SCOTT², D. LI³, J.L. OLIPHANT¹, T.V. TRUONG¹, N.L. PORTER¹

¹Torion Technologies, Inc.

²Idaho National Laboratory

³Brigham Young University

Earlier this year, Torion Technologies introduced an improved version of its GUARDION®-7 field portable GC-TMS system. The system (marketed as the TRIDONTM-9 by Torion and as the GUARDION® by Smiths Detection) has improved analytical performance along with increased ruggedness. Like its predecessor, the new system continues to take advantage of SPME sampling and sample introduction. Concurrent with the development of this next-generation GC-TMS, has been the development of a suite of sampling technologies that can assist in acquiring samples from air, liquids, and surfaces while employing SPME sampling technology. For each type of sample, new strategies to improve the extraction and collection of targeted compounds. In one case, a portable field vacuum extractor (FVE), developed at Idaho National Laboratory and under prototype hardware development at Torion allows increased sampling efficiency for the SPME collection of semivolatiles from surfaces by providing a low vacuum environment over the surface during sampling by the SPME fiber. Increased sample collection results in shorter sampling times using this approach as demonstrated for several Chemical Warfare Agent (CWA) simulants. To support in-field calibration and quantitation applications, a constant headspace concentration calibration vial has been developed. This approach encapsulates the desired calibrants in cross-linked, micro-ground PDMS particles, which for a given temperature, bleed into the headspace at a constant level allowing hundreds of quantitative samples to be acquired. For the detection of biological threats, a prototype, portable, and automated chemical processing unit designed to liberate unique, small molecule biomarkers from bacteria (at this stage, *Bacillus anthracis* spores have been targeted). These small molecule biomarkers are then sampled onto a SPME fiber, which is subsequently analyzed by GC/MS. Finally, a small-format, in-needle sample concentrator housed in the same form factor and dimensions as the SPME needle is under development for the concentration of trace analytes.

The Sample Analysis at Mars (SAM): Developing Analytical Tools to Search for a Habitable Environment on Mars

D. HARPOLD

NASA/GSFC, Greenbelt, MD

NASA's next exploration mission to the surface of Mars, the Mars Science Laboratory (MSL), is scheduled to be launched in late November 2011 and will land on the Mars surface in August 2012. MSL's rover, named Curiosity, will operate on Mars for at least one Mars year (approximately two Earth years) and explore and quantitatively assess the habitability of the region by measuring any complex organic molecules as well as isotopic composition of inorganic and organic carbon that may be present in rocks and soils. One of the scientific instruments on board Curiosity is the Sample Analysis at Mars (SAM) instrument suite consisting of a Quadrupole Mass Spectrometer (QMS), a Gas Chromatograph (GC) and a Tunable Laser Spectrometer (TLS). The QMS and GC can operated together in a GCMS mode. The TLS obtains precise isotope ratios for C and O in carbon dioxide and measures trace levels of methane and its carbon isotopes. This presentation will focus on some of the engineering challenges facing the SAM team during the development stages and thru the integration and delivery of the suite to the Rover.

Applications of Field-Mobile Purge and Trap GC/MS for Onsite Water Analysis

G. PATTERSON, C. LIU, M. WELLS, D.J. BARKET

FLIR Mass Spectrometry (Griffin), West Lafayette, IN

There is an increasing interest from certain sectors of analytical chemistry, including the environmental and forensic analysis communities, for instrumentation that can make measurements on-site, at the point where the samples are collected. On-site analysis can save time and money, preserve valuable chemical information, and provide immediate information in critical situations. Water samples in particular are of importance in environmental applications, and can benefit significantly from immediate on-site analysis. A simplified, ruggedized purge and trap module that directly interfaces with a mobile GC/MS has been tested to determine its capability for analyzing organic pollutants in water.

The ruggedized purge and trap module was interfaced to a Griffin 460 mobile GC/MS system through the Universal Sampling Port, which is included on that instrument for interfacing various sampling accessories. The purge and trap was designed to mate directly to the port for both gas and electrical connections. Methods were developed using specific purge and trap control software written into the Griffin System Software package. Purge and trap parameters including purge flow, purge time, and GC temperature program were all optimized for the individual analyses described below. Samples were prepared via dilution into distilled water from analytical standards generally acquired from Aldrich and Accustandard. The purge and trap module was tested against a variety of relevant organic samples in water, including VOCs and disinfection by-products in drinking water from various sources.

Oil-in-Water Monitoring in the North Sea using Membrane Inlet Mass Spectrometry

B.BRKIC, N.FRANCE, J.SREEKUMAR, K.THABETH AND S.TAYLOR

University of Liverpool and Advanced Sensors Ltd, Liverpool, UK.

A membrane inlet mass spectrometry (MIMS) system has been used for detection and analysis of two types of North Sea crude oil. The system was installed on-field on the Flotta Oil Terminal (Orkney, UK). It consisted of a quadrupole mass spectrometer (QMS) connected to the capillary probe with a silicone-based membrane. The produced mass spectra and calibration plots from the MIMS instrument showed capability to measure levels of individual hydrocarbons within crude oil in sea water. The generated mass spectra from the field tests also showed ability to distinguish between different types of oil and determining concentrations of toxic hydrocarbons in oil (e.g. benzene, toluene and xylene (BTX)). The performance of the instrument at different temperatures of sea water and oil droplet sizes was also investigated. The results showed that QMS-based MIMS system has a potential to complement existing oil-in-water (OiW) monitors by being able to detect different oil types and specific hydrocarbon concentrations with high accuracy, which are currently not supported in commercially available OiW monitors.

Magnet Portable Mass Spectrometer for Direct Control of Gases in Sea Water

A. ANTONOV, V. KOGAN, D. LEBEDEV, A. PAVLOV, Y. CHICHAGOV, S. VLASOV

A.F. Ioffe Physical Technical Institute, Academy of Science, St. Petersburg, Russia

Portable automated magnet mass spectrometer with membrane inlet system for direct control of alkanes (C1-C5) and air constituents in seawater surface layers were considered. Characteristics, structure, main units and operating modes of the instrument were described. The dynamic peculiarities of the instrument response on target compound introduction were determined and taken into account at operating modes optimization. The results of testing of the direct mass spectrometric determination of air constituents, methane, ethane, propane, isobutene and pentane in water samples for fitful and permanent operating modes were discussed.

Mobile High-Resolution Multiple-Reflection Time-of-Flight Mass Spectrometer for in-situ Analytics

Student Abstract Award Winner

J.LANG, W.R.PLAß, T.DICKEL, J.EBERT, H.GEISSEL, M.YAVOR, C.SCHEIDENBERGER

Giessen University / GSI, Germany

Many mass spectrometric methods, such as de-novo sequencing, require high mass resolving power and accuracy to determine unambiguously the composition and structure of molecules. Until now, mass spectrometers for these applications are rather large and immobile.

In this contribution a novel and mobile multiple-reflection time-of-flight mass spectrometer (MR-TOF-MS) will be presented. It will achieve a high mass resolving power exceeding 100000 and sub ppm accuracy in a compact design. Due to short cycle time (compared to FT-ICR and Orbitrap MS) vacuum requirements are rather moderate and the measurement rate up to 1kHz provides GC/MS compatibility. There is no fundamental upper mass limit and a large duty cycle allows for high efficiency. Its compactness and robust concept favors in-situ analytics at any place, even in an rough environment. Mechanical stability has been carefully considered to obtain a rugged setup in every component. An atmospheric pressure interface (API) for atmospheric ionization techniques (DESI, ESI, REIMS) makes it versatile and opens various fields of application. Besides the API the MR-TOF-MS consists of an RFQ cooler, RF ion trap, time-of-flight analyzer, MCP detector and DAQ. Vacuum system components, power supplies as well as electronics are mounted together with the ion optical mass spectrometer parts in a single frame. The system has been built and is currently being commissioned.

Projected applications include in-situ mass spectrometry such as realtime tissue recognition in electrosurgery, identification of mycotoxins and analysis of soil samples for environmental studies. This unique combination of high mass resolving power and accuracy, compactness, robustness and mobility perfectly qualifies for use in harsh environment, future space missions or airborne climate investigations.

New Person Portable Gas Chromatograph for Harsh Environments – Design Criteria, and Verification Testing

C.S. SADOWSKI¹, J.L. JONES¹, E.D. LEE¹, E.G. DIKEN², and D.D. MANNING²

¹*Torion Technologies, American Fork, UT*

²*Smiths Detection, Danbury, CT*

Torion Technologies and Smiths Detection have developed, designed and fielded the next generation field portable gas chromatograph–mass spectrometers (GC-MS). Based on the Toroidal MS technology employed in the Torion GUARDION®-7, the new instrument has been designed for use in harsh environments, improving the performance, operational simplicity and expanding the applications. The GC-TMS system is capable of operating in temperatures ranging from zero to 45oC and has been sealed for use in chemically contaminated environments. The system has been ruggedized to withstand transport, handling and for use in harsh environments, illustrated, for example, by operation at drill rig sites, rapid environmental site assessment at hazardous waste sites, and use by deployed troops and first responders. Meeting the challenges of size and weight reduction, while maintaining operational capabilities and improving performance, required detailed attention to all aspects of the design. Managing internal temperatures and meeting the design criteria for size and weight were the prime challenges faced during the design process.

The use of computer aided design tools for heat management and ruggedization provided for rapid simulations that helped guide the design process. Verification that design criteria were met required that extensive testing be performed. Test criteria and results for the following will be discussed in this presentation:

1. Environmental
 - a. Temperature - operational and storage
 - b. Humidity and rain
 - c. Sand and dust
2. Physical
 - a. Shock and vibration
 - b. Chemical contamination and decontamination
3. Performance
 - a. Gas chromatograph
 - b. Mass analyzer
 - c. Total System

Development of a Miniature Rectilinear Ion Trap Array with Independently Controlled Channels

¹P. HENDRICKS, ²J.D. MAAS, ²W.J. CHAPPELL, ¹R.J. NOLL, ³Z. OUYANG, ¹R.G. COOKS

¹Purdue University, Department of Chemistry, West Lafayette, IN

²Purdue University, Department of Electrical Engineering, West Lafayette, IN

³Purdue University, Department of Biomedical Engineering, West Lafayette, IN

An eight-channel array of miniaturized rectilinear ion traps (RIT) with electrically isolated electrodes has been constructed using stereolithography (SLA) technology. The trapping dimensions for each channel measure 1.66 x 1.33 x 16.66 mm, X0, Y0, and Z respectively, and are arranged in a circular pattern around a single central detector. The array is metal plated through uniform electroless Cu deposition, and then subject to metal ablation using a high aspect ratio laser for electrical isolation of each electrode. Using bias tee networks and dedicated operational amplifiers individual ion trap control can be used to improve the overall spectral quality of the device by compensating for dimensional variation of between ion trap channels. The device is operated using a discontinuous atmospheric pressure interface (DAPI) for direct sampling of externally generated ions therefore operated at pressures of ~10⁻¹ to ~10⁻² Torr during sample introduction and at the start of mass analysis. Single channel performance for mass spectral resolution is approximately 1 to 2 Th FWHM across the mass spectrum and detection of chemical species in excess of m/z 1000 is demonstrated. Due to the miniaturized size, low amplitude voltages can be utilized for the RF. Detection of the entire charge state envelope (+14 to +26) for intact proteins such as myoglobin (17 kDa) was completed at RF amplitudes of less than 1500 Vp-p (950 kHz drive RF). Additionally, improved sensitivity and dynamic range of 0.1 ug/ml to 10 ug/ml propranolol is demonstrated through parallel operation of multiple ion traps and tandem MS.

Redesign of the VAPoR Miniaturized Pyrolysis TOFMS for Improved Sensitivity

A.E. SOUTHARD, S.A. GETTY, D.P. GLAVIN, C.A. KOTECKI, S.H. FENG

NASA Goddard Space Flight Center, Greenbelt, MD

We are developing the VAPoR (Volatile Analysis by Pyrolysis of Regolith) instrument to study gases evolved from regolith during upcoming NASA analog field campaigns and future robotic or human missions to the Moon, asteroids, and Mars. VAPoR can heat powdered rock samples up to temperatures of 1300°C and analyze the water, organic compounds and other volatiles released from solid samples by time-of-flight mass spectrometry. Recent efforts to improve the electron beam current emitted from our carbon nanotube field-emission source have led to the development of a larger emitter and redesign of the ion source geometry. These efforts lead to orders of magnitude higher beam current. This beam current will provide greater sensitivity with the introduction of a larger microchannel plate detector in the future.

Currently, the time of flight mass spectrometer can be used in two modes with or without a gridless reflectron enabling us to optimize the ion spectrum for mass resolution or sensitivity. Modeling using SIMION indicates an expected mass resolution of 500 given assumptions about the geometry of the ionization volume and initial kinetic energy distribution. Efforts are underway to reach this resolution target by optimization of the extraction voltages, pulse times, and reflectron fields. Until now, we have achieved a mass resolution of 270. Our current geometry offers excellent shielding of fringing fields associated with the electron beam focusing in the ion source but sacrifices spatial focusing ability of the ions formed. Still, spatial focusing appears to be a less significant source of error.

Recent Advances in Portable Mass Spectrometry Systems at Kennedy Space Center

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Portable mass spectrometer systems provide a wealth of information when troubleshooting equipment. One of the primary challenges of mass spectrometry is the ability to transport the system to the equipment. This presentation will provide a variety of examples of unique solutions to solve many operational needs for mass spectrometry at NASA's Kennedy Space Center. Examples will discuss system portability, ruggedness, sampling properties. Individual components comprising the systems will be discussed so as to evaluate their effectiveness. Focus will also be placed on the ability to quickly modify the hardware for various applications. Finally, attention will be brought to the importance of a generalized software platform in achieving the many needs of portable field analysis.

Cylindrical Toroidal Ion Trap Mass Spectrometer

D. AUSTIN, N. TAYLOR

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We present a new ion trap mass analyzer employing a toroidal geometry, in which cylindrical electrodes are used rather than the hyperboloidal surfaces of revolution used in conventional toroidal ion traps. Analogous to the cylindrical ion trap (CIT) and the rectilinear ion trap (RIT), the cylindrical toroidal trap represents a simplified electrode geometry facilitating miniaturization or multilayer microfabrication. The toroidal geometry provides a large trapping volume, needed to maintain sensitivity in a reduced-size analyzer. Asymmetric overlap of the electrodes creates the proper fields, overcoming the inherent asymmetry of the toroidal geometry. Adjustment of the electrode spacing allows control of higher-order field components, and allows different ratios of major to minor radii. Miniaturization takes place as the minor radius is reduced (the characteristic trapping dimension) while holding the major radius at a large value. Ions are ejected radially onto a single point, allowing a small detector or a single detection wire to be used. Preliminary data from a full-sized prototype demonstrate device function on several organic compounds.

Design and Use of Portable and Compact Sampling Systems for Mass Spectrometers

K. WRIGHT

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Residual gas analyzers (RGA's) are most commonly installed on vacuum systems to monitor system performance and to be use as a diagnostic tool when problems arise. While the original purpose of RGA's was residual gas analysis their role has evolved and their utilization for process monitoring and gas analysis has increased. Since many applications requiring gas analysis take place at pressures higher than optimal for linear quadrupoles, the most common type of RGA, it became necessary to incorporate RGA's into compact sampling systems with integrated vacuum pumps.

Operational theory and design choices for compact sampling systems will be discussed. Ion source choice ("closed" *versus* "open"), mass range, vacuum pumps, sampling configurations, and detector choices (EM *versus* Faraday) will all be presented. Also, relevant specifications commonly used to describe RGA performance: minimum detectable partial pressure (MDPP), resolution, sensitive, linearity, zero blast, abundance sensitivity, measurement speed and peak stability will be defined while highlighting the analytical figures of merit that are most relevant for compact sampling systems. Products from INFICON Inc and Pfeiffer Vacuum including the Transpector CPM, Ecotec E3000, HAPSITE ER, PV Star/ThermoStar, and related products will be used as examples to highlight a variety of applications that include: semiconductor process monitoring, leak detection, CWA (TIC's & TIM's) detection, thermobalance monitoring, and oil/gas exploration.

Design of Pocket Mass Spectrometer in a Mobile Phone Size

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In sequel to the development of Palm Portable Mass Spectrometer (J. Am. Soc. Mass Spectrom. 2008, 19, 1442–1448), a new design of pocket mass spectrometer in a mobile phone size is proposed. The technologies for shrinking mass spectrometer include miniaturized high vacuum system with sample gas concentration and separation, mass spectrometer control chip, cold electron ionization, and miniaturized DC power supplies, etc. Adsorption and desorption on a surface promises the sample gas concentration of up to 1,000 times, enhancing the detection limit of trace chemicals in the air. Micro-GC with a pulsed gas introduction is expected to separate and concentrate the various gases in the sample. Mass spectrometer control circuits integrated in a microchip certainly will save the battery power, size, and weight. Cold electron source for sample gas ionization is also intriguing. A secondary electron multiplier initiated by photons seems to generate more electron current than a field electron emission. Since an ion trap mass spectrometer requires various voltages for printed circuits, electron gun, electron acceleration, RF high voltage generation, and high voltages for ion detector and ion getter pump, reducing the size of DC/DC converters that supply those voltages from a battery requires another challenge. Instead of ramping RF high voltage for mass scanning in an ion trap, frequency modulation is preferred with low voltage, which would be appropriate for mass spectrometry in a sprite discharge environment. Plausible and available techniques for the design of pocket mass spectrometer and some of the interested potential applications are discussed.

A Completely Handheld Ambient Ionization Source for Mass Spectrometry Based on a Low-Temperature Plasma (LTP)

Student Abstract Award Winner

J.S. WILEY¹, J.T. SHELLEY², S. SOPARAWALLA¹, R.J. NOLL¹, G.M. HIEFTJE², R.G. COOKS¹

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A novel adaptation of the Low-Temperature Plasma (LTP) ambient ionization source has been developed and coupled to a miniature mass spectrometer, offering portability for true in-field analysis. Advantages of low gas and power consumption as well as no solvent usage have aided in developing the field-ready, handheld device for trigger-based, “point-and-shoot” sampling/ionization. A small lithium polymer battery was used to power a home-built circuit within the device, which provided ~2 kV ac to ignite a dielectric-barrier discharge in either helium or air. The excited species from the plasma are capable of directly interacting with gaseous, liquid or solid samples, resulting in sample desorption/ionization.

Analytical figures of merit for a few classes of compounds (mainly pesticides, explosives and drugs of abuse) under various operating conditions will be presented. In particular, the performance of conventional LTP versus handheld LTP has been evaluated, interestingly yielding increased performance for handheld LTP. An increase in proton transfer ionization was observed when the air discharge gas was replaced with helium (from a small He cartridge). However, the formation of nitrate adducts, as occurs with many explosives, was found to occur roughly the same extent with both gases.

The reduced gas flow rates and electric fields exhibited by handheld LTP have enabled a smoother coupling to mini MS when compared with conventional LTP. Initial results have indicated superior sensitivity, without the use of supplemental pumping, for the analysis of analytes in neat solution and complex mixtures. Results for the long-distance transfer of sample ions from the ionization region to the MS inlet will also be presented, illustrating the full advantages and potential of a handheld ambient ionization source.

A Miniaturized Laser-Ablation Mass Spectrometer Designed for In-Situ Measurements on Planetary Space Missions

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The in-situ analysis of extraterrestrial material onboard planetary rovers and landers is of considerable interest for future planetary space missions. With spectroscopic instruments, e.g. α -particle X-ray spectrometers, γ -ray spectrometer, flown on previous spacecrafts it was due to their low detection sensitivity only possible to measure major elements and no isotopes in solid state material. However, for the further understanding in the formation and evolution of solids in our planetary system a deeper investigation into minor and trace elements is essential. High accuracy and sensitive measurements on bio-relevant trace elements, i.e., sulphur or phosphorus and others, play an important role in the field of astrobiology. Anomalies in isotopic pattern of bio-relevant elements found on planetary surfaces can be useful for the identification of possible past and present extraterrestrial life. Age dating of solids can be achieved by a detailed analysis of isotopic pattern of radiogenic elements.

In this respect our group has designed a self-optimizing miniaturized laser ablation time-of-flight mass spectrometer (LMS) of reflectron type for future space applications. An Nd:YAG laser with 266nm wavelength, pulse length of 3ns and a repetition rate of 20Hz is used to ablate surface material. The beam is focused within 20 μ m onto the sample and more than 100 GW/cm² can be achieved. The instrument with a length of only 120 mm, a diameter of 60 mm and a weight of about 500gr (all electronics included) has with a typical resolution of

$m/\Delta m \sim 600$ and the high dynamic range of about 10^7 a similar performance than large laboratory systems. Furthermore, the more than ten voltages applied on the instrument and the laser fluence are computer optimized by using a self-written software based on a swarm, scanning algorithms respectively. High accuracy, sensitive, and reproducibility measurements in sub-ppm range are therefore possible.

Autoresonant Ion Trap Mass Spectrometry (ART MS)

G.A. BRUCKER, G. J. RATHBONE

Granville-Phillips Vacuum Products, Brooks Automation, Inc., Longmont, CO

ART MS technology was first disclosed at the 7th Workshop on Harsh Environment Mass Spectrometry. Small size, fast sampling, low power consumption, light weight and rugged construction make ART MS technology the ideal candidate for in-situ mass spectrometry in a wide variety of remote gas analysis applications including harsh sampling environments. We will explain the principles of operation of ART MS instrumentation and compare its operation against legacy mass spectrometry sensors. We will also describe the basic performance specifications of its first commercial implementation, the VQM 830 Vacuum Quality Monitor. The new instrument provides a flexible platform for basic mass spectrometry research as well as fast and easy incorporation into fieldable instrumentation.

Negative Ions for Fieldable Mass Spectrometry

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There are certain analytical situations for which negative ion mass spectrometry has advantages over the more commonly used positive ion methods. This is especially true for those analyte molecules with high electron affinity that are amenable to electron capture ionization. The purpose of this talk is to show some of the special results that have been obtained for field measurements of two perfluorinated molecules, perfluoro dimethylcyclohexane and uranium hexafluoride. The former has potential applications as an airborne chemical tracer in the environment, the latter finds use in uranium isotope enrichment. Despite the wide disparity in chemical reactivity of the two molecules, the negative ion mass spectra of both show a high discrimination against background interference and high stability of the molecular ion relative to the positive ion formed by electron impact.

This research has been supported by Tracer Detection Technology Corp. and by the U.S. DOE Office of Nonproliferation and International Security.

Mobile Mass Spectrometer in Daily Use – Experiences Made by Non-Scientific Operators

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E²M (Enhanced Environmental Mass Spectrometer) is a compact robust quadrupole mass filter with a membrane inlet, designed for mobile application. The ruggedized instrument can be installed on a vehicle and run from the vehicles power supply. Typical applications are environmental protection, mobile on-site analysis, event monitoring, first responders or homeland defence. The instrument affords reliable identification of organic compounds in solid, liquid or gaseous samples. The almost direct inlet via an air/surface probe provides fast results in monitoring modes. Even though combined with a gas chromatograph over the complete E²M system delivers a versatile field deployable GC/MS capability. Non-complicated controls and data acquisition enhance the instruments ease of operation. Data evaluation is fully automated.

The effective use of the system by any kind of first responders will be shown. Successful integrations in different types of vehicles and the use in a ship air monitoring system will be demonstrated. Also data resulting from the typical use of customers are presented. Several representative examples for the useful application of the system e.g. the identification and localisation of an agent at a poison attack in a pub or the contamination of an open water recreation area made by fire fighters or other first responders will be shown. Additionally recent enhancements and new applications will be presented.

Utilization of Lightweight MS based Instrumentation and Small UAV Platforms for In-Situ Volcanic Plume Analysis

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We describe the joint research effort to develop low-cost, field-deployable airborne platforms and integrated in-situ MS based sensing instrumentation to perform in situ volcanic plume analysis in conjunction with orbital assets to validate state-of-the-art models of plume transport and composition.

Current remote sensing retrieval and transport modeling efforts to detect, characterize, and track airborne volcanic emissions suffer from very sparse in situ validation data. Ash and gas concentrations derived from analysis of satellite remote sensing data, with rare exception, remain essentially invalidated by in situ data. Given recent European aviation experience after the 2010 Icelandic eruption and past near-fatal aircraft ash encounters, basic assumptions of plume chemical and physical processes, and the boundary conditions for both mass retrieval and trajectory prediction models, are being called into question. In view of the hazardous high-risk flight environment posed by volcanic clouds, the use of small unmanned airborne vehicles (UAVs) to validate SO₂ and ash concentration and mass retrievals from orbital multi-spectral infrared sensor data is appropriate.

Using Costa Rican volcanoes as a natural laboratory and different airborne platforms including small unmanned aerial vehicles (sUAV) and tethered balloons; several gas sensors including the ULISSES miniature mass spectrometer system combined with temp, pressure, relative humidity and GPS data are being lab tested and field deployed into the active plume of Turrialba Volcano while collecting near remote sensing data (UV, IR) and satellite remote data.

A Transportable FTICR/MS for Direct and Real-Time Analysis of VOC Contaminants in Air and Water

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A transportable FTICR/MS has been developed based on a permanent Halbach magnet. The magnet is 1 to 1.5 T. The resolution is better than 0.03 Da in the 2-500 mass range. Ionization is conducted inside the ICR cell by ion-molecule reaction. Precursors for chemical ionization are chosen to achieve good selectivity towards specific compounds of interests and to avoid reactions with the molecules constituting the matrix (such as N₂, O₂ or H₂O). H₃O⁺ was shown to react with most volatile organic compounds, and CF₃⁺ with the halogenated compounds such as chlorofluorocarbons and hydrochlorofluorocarbons. Moreover, as reaction conditions are well controlled direct and reproducible quantification of molecules identified in the gas is possible. The transportable FTICR/MS, developed jointly at LCP and AlyXan, has proven useful for in-situ analysis of ambient gases. A few examples will be shown, such as analysis of exhaust fumes, polymer degradation and plasma analysis. A specific harsh environment FTICR/MS was developed by AlyXan for analysis in submarine atmosphere, to monitor contaminants of the air breathed in by the crew. More recently the FTICR/MS was associated to a membrane introduction system (MIMS) for water analysis. MIMS is used both as a barrier between the water sample and the vacuum cell and as a concentrator of the sample. The membrane showed enrichment factor of more than 1000 for volatile non-polar compounds and around or less than 10 for soluble compounds. A complex solution was studied, and the results will be shown.

Low Power Atmospheric Gas Sampling System Based on ART MS Sensor and NEG-Ion Pump System

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¹*Granville-Phillips Products, Brooks Automation, Longmont, CO*

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The combination of an ART MS gas analyzer with a dual-technology vacuum pump consisting of a non evaporable getter (NEG) and a small size ion pump provides a very compact and low power gas sampling system for remote sensing applications. The ART MS sensor technology provides the advantages of very low power requirements, compact design, fast scanning, ruggedness and sensitive gas detection. The NEG-Ion pump provides very large pumping speeds and gas capacity, a total pressure reading, low power consumption, vibration free operation and an unprecedented small size that perfectly matches ART MS sensor form factor. Several different atmospheric gas sampling schemes are discussed and the effect of differential pumping speeds on partial pressure levels are analyzed.

A Software Package for Mass Spectrometer System Operation, Trouble Shooting and Prototyping

C.R. ARKIN, C. CURLEY, D. FLOYD, D. LUCAS

Engineering Services Contract, Kennedy Space Center, FL

A PC-based software program has been controlling the mass spectrometer systems used to launch the Space Shuttle since 2000. This software program has expanded to support several mass spectrometer systems since that time; however, the software was designed to interface with an embedded computer system which perform the command and data acquisition. Recently this software package was ported such that only a PC is required, and has expanded in flexibility to interface with a variety of mass spectrometer system end items such as mass analyzers, turbo pumps, ion gauges, mass flow controllers, pressure transducers, and the like. This software package, known as the Analyzer Control System (ACS), integrates a variety of end items into a single user interface allowing consistent data presentation, real-time data manipulation (view data in parts-per-million, etc), integrated data storage with consistent time stamps, timed events via scripting and much more.

A High Density Micro-Ion Trap Array Miniature Mass Spectrometer

¹T. WU, ²A. CHAUDHARY, ¹J. WANG, ²F. VAN AMEROM, ²R.T. SHORT

¹University of South Florida

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We report on a novel approach to develop a high density μ -cylindrical ion trap (HD μ -CIT) array mass spectrometer (MS), with emphasis on reducing the device capacitance, optimizing trap geometry and sensitivity, and improving component alignment to extend the mass range and improve the mass resolution. Microelectromechanical system (MEMS) technologies are used to fabricate the ring and endplate electrodes with micron scale precision. A hexagonal orientation of CITs was adopted to pack more μ -CITs per unit silicon (Si) volume. μ -CIT geometries with a range of radii (r_0) (250 - 350 μm) were investigated in SIMION to determine the optimum z_0/r_0 ratios. To reduce the device capacitance and increase breakdown voltage, a range of spacings between ring and endplate electrodes (up to 60 μm) were also investigated through simulations. Designs for optimum geometries were incorporated in an optical mask for MEMS fabrication. Deep reactive ion etching (DRIE) and potassium hydroxide (KOH)-based etch methods were used to batch fabricate multiple μ -CIT arrays in a single Si wafer. Capacitance between the ring and endplate electrodes was reduced by selectively etching the sputtered metal layers. A package for easy assembly and connections of μ -CIT components was designed and fabricated in Ultem, a transparent plastic material compatible with high vacuum operation. Design of a vacuum system with provision for differential pumping and simultaneous ionization of analytes in all traps in a μ -CIT array is underway. A microchannel plate (MCP) coupled with a multi-anode plate will be used as the ion detector, allowing investigation of the performance of each μ -CIT separately. It is expected that the new design of HD μ -CIT array MSs will provide much higher sensitivity than previously realized. The results obtained from these experiments will help lay the design foundation for the next generation μ -MS systems, paving the way toward a low power handheld chemical analyzer.

Development of a MEMS Mass Spectrometer Based on TOF Architecture for Gas Analysis

C-M. TASSETTI, L. DURAFFOURG, J-S. DANIEL, T. LAGUTERE, F. PROGENT

CEA DAM-DIF, Arpajon, France.

The main purpose of our project is to develop a small dimensions mass spectrometer for gas analysis suitable for harsh environment on the field applications. The mass spectrometer will be connected to a gas micro-chromatograph that has been developed specially for this project. Due to their high operating rate, Time Of Flight (TOF) mass spectrometers have been used efficiently in gas analysis. In its basic form, TOF architecture is made of an ion source, an acceleration zone and a drift zone where ions are separated by the ratio of mass to charge (m/z). Some parasitic dispersion, such as ion's energy dispersion or ion's spatial dispersion, could reduce drastically the mass spectrometer's global performances. The TOF architecture's efficiency could be enhanced by adding a reflectron. It is a challenge to downscale the electrostatic mirror and design it using MEMS technology.

A Study of How Alternative Buffer Gases can Affect Energetic Material Detection in an Ion Trap Mass Spectrometer

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Due to their inherent nature, energetic materials are more reactive than the traditional hydrocarbons and are better able to undergo the substitution of one or more groups located in the alpha position to the electron withdrawing nitro group. The mass spectra of various high explosives were determined using electron ionization and an ion trap containing nitrogen gas. The spectra obtained displayed characteristic fragmentation in accordance with their respective structures. When the nitrogen gas was replaced with labile deuterium gas, the spectrum for certain compounds of interest showed an increase in the M+1 and M+2 peaks indicating whether the compound had been mono or di-substituted with deuterium. Due to the small potential well on the miniature ion traps and the ability to undergo many neutral collisions, it is an ideal environment to couple chemistry with ion fragmentation to reduce false positives in the spectrum. As hydrocarbons and even some energetic materials do not undergo these substitutions, one can rapidly test (1-2 minutes) for a specific group of high explosives by identifying the M+1 and M+2 peaks. The ideal high explosives are stable enough to undergo electron ionization and substitution without completely decomposing, yet not so stable that they do not substitute at all.

Pulsed LIBS Ablation System with Static High Resolution Quadrupole for ^3He Determination

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The analysis of ^3He from tritium decay in metal surfaces exposed to large amounts of tritium gas is used to study material lifetime of potential fusion reactor components. To minimize the amount of exposure and facilitate sample handling, the analysis system needs to be designed to handle small samples with extremely high sensitivity. Savannah River National Laboratory is currently assembling a new static mass spectrometer based on a combination LIBS/Laser Ablation system interfaced to an ultrahigh static vacuum system. The vacuum system uses a combination of a gated turbo pump system with isolated ion getters and direct ionization pumps. The vacuum chamber is directly interfaced to a high resolution Extrel MAX60 quadrupole which is optimized for the separation of ^3He from HD. The quadrupole has a high gain SEM detection module for ppb level sensitivity in micrograms of ablated sample. The getter is designed to trap residual tritium and other hydrogen components that might be present. The sample is mounted on a small bellows sealed positioning stage that may be raster across the laser. The laser is a Quantel Brilliant EaZy NdYAG set for 1064 nm operation and focused to about a 50 micron ablation spot size. Harmonic doublers may be used to work at lower wavelengths and sharper spots. The beam is focused through a quartz or sapphire window and may be adjusted due to the use of infinity correction optics and standoff 100 mm objective in the beam design. A splitting hot mirror allows the focal point to be monitored using a CCD camera. The beam is maintained in a closed system.

In line Nafion-based water gas remover for In Situ Mass Spectrometry

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For over a decade membrane inlet mass spectrometer (MIMS) have been adapted to quantify in situ the dissolved gases in sea water at a great variety of depth (eg. Short et al, Meas. Sci. technol, 1999). Polydimethylsiloxane (PDMS) membrane are widely used because of the variety of gases permeating through it. The amount of water gas permeating through PDMS is however rather high. Higher pumping rate and decrease in instrument sensitivity result from the high water partial pressure. Cold traps have been used to cope with this problem (Schülter and Gentz, J. of Am. Soc. Mass. Spec., 2008), but are impractical/high power demanding for long term in situ mass spectrometer (MS) deployment. Molecular sieve is efficient in binding water, even in vacuum, but binds hydrogen sulfide as well. We therefore developed a drying module based on molecular sieve beads in a vacuum chamber. The gas sample coming from the membrane inlet passes through the chamber in a nafion tubing before entering the ionization chamber of the MS. This module achieves a 5 time reduction in the water partial pressure, without reducing the other gases partial pressure. The system sustained its performance for about 4 days of continuous use before the water removal efficiency decreased. Backing off the module proved to restore the water removal efficiency. In addition, the hysteresis of the other gas signals observed when pressure cycling the inlet (a known problem with PDMS membrane) appears to be reduced by the use of the drying module.

Differential Mobility Ion Pre-filter for Field - Deployable Atmospheric Pressure Ionization Mass Spectrometers

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Detection of target chemicals in complex environments such as public spaces (for example, administrative buildings, shopping malls and subway systems) is problematic when utilizing atmospheric ionization (API) mass spectrometry (MS). This is mainly due to complex gas phase processes, which lead to the formation of a large number of ionic species and their cross interactions in the ionization region. The presence of numerous interferences in such environments increases the false alarm rates, frequently to unacceptably high levels. An effective method to avoid these challenges is to combine MS with other fast-operating separation methods. This approach enhances the detection accuracy of the system as a result of: (a) selection of targeted ion species before introduction in the MS and (b) providing additional orthogonal chemical information for targeted species.

Planar Differential Mobility Spectrometry (DMS) is a rapid ion separation method, which can operate as a standalone spectrometer which can provide mobility spectra for positive and negative ion species or as a continuous ion filter for targeted ion species. In the latter case, DMS can be tuned for filtration of selected ions of interest and for effective removal of other undesirable interferences ion species prior to analysis by MS.

AB SCIEX recently released their SelexION™ Technology device which provides planar DMS pre-filtering capability to their Triple Quad™ 5500 and QTRAP® 5500 laboratory mass spectrometer systems. The SelexION™ device provides proven improvements in scan speed, tuning stability, separation power (through the use of chemical modifiers), reproducibility and robustness, and chemical noise reduction. In this poster, we will present design concepts and expected benefits of using planar DMS as a pre-filter for miniature MS. The proposed designs are intended to operate with various types of fieldable API-MS systems equipped with capillary inlet sample introduction. Progress towards development of such a system will be presented.

Performance Enhancement for Miniature QMS Through Application of a Magnetic Field

Student of Note

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One of the challenges of deploying miniature mass spectrometers (MS) in harsh environments is that of reducing the size (to render the MS system portable), whilst at the same time maintaining instrument performance in terms of MS resolution, sensitivity and mass range. Previous work has identified that application of a static magnetic field can improve the resolution of a miniature quadrupole mass spectrometer (QMS) and this simple method of performance enhancement offers advantages for field deployment. The magnetic field may be applied transversely (radially) to the quadrupole mass filter (QMF) or axially and performance improvements have been observed experimentally in both cases. The experimental results have been successfully simulated on the basis of our QMS model, which computes the individual trajectories of large numbers of ions (typically 108) injected randomly into the QMF. Mass spectra may be obtained for a range of applied voltages (U/V), electrode length and inscribed radius (r_0), RF frequency and ion energy. We have recently adapted our QMS model to allow simulation of any electrode geometry (circular, square or hyperbolic) and configuration. The program now allows instrument simulation not only for the range of conditions above but also allows r/r_0 ratio to be specified. The program allows electrodes to be misaligned or displaced so as to examine the effect of manufacturing tolerances on QMS performance. We present here the results of recent instrument simulations for two HEMS application areas: (i) detection of low mass isotopes ($1 < m/z < 6$ Da) and (ii) detection of $^{12}\text{C}/^{13}\text{C}$ for medical diagnosis.

The Development of Condensed-Phase Membrane Introduction Mass Spectrometry (CP-MIMS) for the Direct Online Analysis of Polar, Low Volatility Analytes from Complex Matrices

Student of Note

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Condensed-phase membrane introduction mass spectrometry (CP-MIMS) uses a semi-permeable membrane to separate an aqueous sample from a liquid acceptor phase (e.g. organic solvent). The membrane precludes the bulk of the sample, allowing analytes of interest to diffuse across and be directed to an ambient ionization source (e.g. ESI). Having a condensed acceptor phase allows the analysis of semi-volatile/non-volatile and/or polar compounds, those not amenable to 'conventional' gaseous acceptor phase MIMS. Our group has been exploring the development of this technique, finding it suitable for the direct, continuous, on-line, trace level monitoring of a wide range of environmental contaminants and bio-analytes. Presented work was carried out using 10cm lengths of polydimethylsiloxane (PDMS) or Nafion[®] hollow fibre membranes with a methanolic acceptor phase directed to an ESI-MS/MS system. Detection limits and signal response times have been determined for a wide range of analytes encompassing environmental contaminants, pesticides and pharmaceuticals in a number of complicated sample matrices, including undiluted artificial urine. The recent development of portable mass spectrometers with ambient ionization sources will facilitate future applications of CP-MIMS for the real time, online measurement of trace polar, low volatility analytes directly in the field.

The Coaxial Ion Trap: Concentric Quadrupolar and Toroidal Trapping Regions

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We present the design and results for a new radiofrequency ion trap mass analyzer, the coaxial ion trap, in which both toroidal and quadrupolar trapping regions are created simultaneously. The device consists of two parallel ceramic plates, whose facing surfaces are lithographically patterned with concentric metal rings and covered with a layer of germanium. Ions can be trapped in either region, transferred from the toroidal to the quadrupolar region, and mass-selectively ejected from the quadrupolar region to a detector. Ions trapped in the toroidal region can be transferred to the quadrupole region using an applied ac signal in the radial direction, although it appears that the mechanism of this transfer does not involve resonance with the ion secular frequency, and the process is not mass selective. Ions in the quadrupole trapping region are mass analyzed using dipole resonant ejection. Multiple transfer steps and mass analysis scans are possible on a single population of ions (as from a single ionization/trapping event), illustrating the larger ion capacity of toroidal ion trap and possible applications in analyzing transient or dynamic events.

Transportable sector-field MS with ion detector array

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Monitoring concentrations of gaseous fuels or detecting hydrogen and its contaminants can be challenging. The IonCam is a compact GC/MS system based on a double-focusing sector field mass spectrometer of Mattauch-Herzog geometry. This type of MS separates ions of different mass to charge ratio (m/z) spatially and focuses ions of equal m/z simultaneously in a focal plane, thus creating complete mass spectra at all times. To take advantage of this unique feature a modified charge coupled device (CCD), sensitive to electrical charges (IonCCD) has been developed. The ion-CCD allows the collection of all dispersed ions, recording a complete mass spectrum at a rate of up to 350 mass spectra per second. The 2126 discrete detector elements (pixels) as well as the integrated readout circuitry of the detector are sensitive enough to detect ion currents at the "Atto-Amps" level. The compact size of the IonCam limits its mass range to 250 amu but shows superior mass resolution for small masses. Most gaseous contaminants that are common in hydrogen production can be detected without prior separation.

Mass Spectrometer for *In-Situ* Detection of Organics in Martian Soil

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We present details on the objectives, requirements, design, and operational approach of the core mass spectrometer of the Mars Organic Molecule Analyzer (MOMA) investigation on the 2018 ExoMars mission. MOMA is part of the ExoMars rover led by the Max Planck Institute in Germany (PI: Dr. Fred Goesmann). A NASA-Goddard-based team contributes the core ion-trap mass spectrometer and electronics. The MOMA mass spectrometer enables the investigation to fulfill its objective of analyzing the chemical composition of organic compounds in solid samples obtained from the near surface of Mars. Two methods of ionization are realized, associated with different modes of operation, in a single compact ion trap mass spectrometer. The first method uses electron ionization (EI) for analysis of derivatized organic compounds received from a gas chromatograph. The second method uses laser desorption ionization (LDI) for analysis of soil samples for higher mass organic compounds including prebiotic or possibly chemical compounds of biological origin. The stringent mass and power constraints of the mission have led to features such as low voltage and low frequency RF excitation and pulse counting detection. Two different types of ion trap, a 3-D and 2-D linear trap, are under investigation for performance.

Design of the Portable Mass Spectrometric Sensor for Vascular and Endocrine Disease Diagnostics

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Design and testing of the interface systems between the entrance of a portable mass spectrometric sensor and human skin for noninvasive diagnostics of vascular and endocrine diseases with monitoring of transcutaneous (through the skin) gas composition were reported. The description of the interface systems, the operating mode and the factors making an impact on the efficiency of measurement procedure were considered. The transcutaneous gas tensions were evaluated through mass spectrometry gas flow determination at skin surface. The results of testing of the mass spectrometric sensor were presented. The efficiency of mass spectrometry method application was discussed.

PIMMS, an all-purpose micro mass spectrometer

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PIMMS - The fully planar integrated micro mass spectrometer on a small chip of $12 \times 7 \text{ mm}^2$ is composed of a RF micro plasma as an electron source for ionization, Synchronous-Ion-Shield mass separator, a micro-channel plate to multiply the measured current, and a detector (Figure 1). It contains all essential components of a mass spectrometer and it is fabricated in Batch process in MEMS Technology. This turns it into a mobile, field-analysis capable device. It was first described by Hauschild in (HEMS2007).

In order to reach the lowest physical detection limit of 1 m/z (which corresponds to atomic hydrogen), improvements in the geometry of the PIMMS were carried out and optimization of the electronic components driving the SIS was performed. The increased detectable mass range now reaches from 1 m/z to theoretical 1200 m/z . The geometry adaptation has the additional desired effect that the ion transmission was doubled. Additionally the sensitivity of the spectrometer was improved via a new concept of current measurement.

Spectra of methane (Figure 2) and hydrogen (Figure 3) measured with the Planar Integrated Micro Mass Spectrometer (PIMMS) are presented. They demonstrate the capability of the PIMMS to detect ions with low mass-to-charge ratio now starting at 1 m/z and an improvement in sensitivity, so that gases with relative concentrations of $<100 \text{ ppm}$ are now detectable. The improved performance enlarges the application range of PIMMS, e. g. portable leakage detector. These results demonstrate that PIMMS is now an all-purpose applicable, mobile device.

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On-site Analysis of Environmental Air and Water Samples at a SAGD Oil Production Facility (Statoil) in Northern Alberta using MIMS

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A portable ion trap (Griffin 400) was modified to include a He flushed membrane interface. The membrane introduction mass spectrometer (MIMS) was plumbed to enable the analysis of both aqueous and gaseous analytes. Lead acid batteries provided over 10 hours of daily field portability for real-time, on-site analysis of environmental samples in Northern Alberta's oil sands. Data were primarily collected at Statoil's Leismer SAGD (Steam Assisted Gravity Drainage) site in June 2010 and Sept 2010 prior to oil production, and June 2011 just after the site's 1 millionth barrel of oil was produced. For comparative purposes, data were collected at water bodies and air sampling locations adjacent to various surface mining facilities operating near Fort McMurray, Alberta. Both single point (from grab samples) and timeseries data sets were produced. Further, samples of bitumen, steam condensate, and other SAGD reagents were collected from the Leismer production facility for lab analysis. Gaseous samples were infused with deuterated toluene (toluene-D8) via a thermally regulated permeation tube. The toluene-d8 signal acts as an internal standard enabling the operator to monitor instrumental artifacts that may affect signal intensity. MIMS data were correlated with