

## EIGHTH MEASUREMENT AND MONITORING LITERATURE UPDATE

### Addressing Forensic Field Analytical Chemistry Issues

Eckenrode, Brian A. (Forensic Science Research Unit, Federal Bureau of Investigation), Valerie Cavett; Philip A. Smith (Uniformed Services Univ. of the Health Sciences), Gregory Kimm, Gary Hook; Erin Sherry (George Washington Univ.).

The 3rd Harsh-Environment Mass Spectrometry Workshop, 25-28 March 2002, Pasadena, California.

The authors present data from a new GC design that is small, lightweight, and has low power requirements for eventual GC/MS field systems. They have explored the use of field Raman systems and present results from these evaluations. Also, they have experimented with the use of solid-phase microextraction (SPME) interfaced to an IMS for the analysis of headspace organic mixtures, including chemical warfare agents. The practice of "temperature programming" is routinely done by changing the temperature of the oven containing a GC capillary column and heating the circulating air within it. This novel GC design does not require a convective approach to column heating. This new low thermal mass (LTM) column heating design has a high thermal efficiency toroidal wrap that can be programmed at high speed while maintaining low power consumption. Data are presented on the use of this column in a conventional GC oven versus an LTM GC in a performance test for chemical warfare treaty verifications. Mass spectrometric parameters such as sampling time, scan rate, and library matching capability have been evaluated for several different, mostly high, ramping rates. The development of a field-portable, battery-operated Raman system enables the application of this non-intrusive technology to analytical measurement situations requiring reliable identification of potentially hazardous materials in the field. Evaluation of these instrument prototypes will provide feedback necessary to develop the instruments into systems useful for on-site characterization of materials relevant to public or personnel safety and security issues. SPME will be used as a sampling front-end for chemical warfare-related compounds followed by IMS and/or GC-MS detection.

<http://cot.marine.usf.edu/hems/workshop/3rdworkshop/program.htm>

### Airborne Deployment of the Aerosol Mass Spectrometer during the ACE-Asia Field Campaign

Jimenez, Jose (California Inst. of Technology), Roya Bahreini, Richard Flagan, John H. Seinfeld; Hafliði Jonsson (Naval Postgraduate School); John Jayne (Aerodyne Research), Douglas Worsnop.

The 3rd Harsh-Environment Mass Spectrometry Workshop, 25-28 March 2002, Pasadena, California.

The Aerosol Mass Spectrometer (AMS) has been developed to provide real-time quantitative measurement of aerosol size and chemical composition over the 50 nm to 5 micron diameter size range. The AMS was deployed inside the CIRPAS Twin Otter airplane during the ACE-Asia field campaign in the first aircraft deployment for this type of mass spectrometer. The AMS operated unattended, and collected data successfully during 15 out of 19 Twin Otter flights. This paper describes the main challenges encountered in this deployment and the strategies used or planned to overcome them. The ACE-Asia field experiment was designed to characterize how particles emitted in eastern Asia (China, Korea, and Japan) affect climate through both direct and indirect radiative forcing. The submicron aerosol was present in discrete layers about 0.5-1 km deep, separated by layers with much lower aerosol mass concentration. Sulfate was a major aerosol component during all flights, and its size distribution was remarkably constant by days and atmospheric layers. Ammonium, nitrate, and organics were also observed in the aerosol.

<http://cot.marine.usf.edu/hems/workshop/3rdworkshop/presentations/Jimenez/index.htm>

Airborne Laser Induced Fluorescence Imaging. Innovative Technology Summary Report  
U.S. DOE, Office of Environmental Management.  
Report No: DOE/EM-0427, 21 pp, Jun 1999

Laser-Induced Fluorescence (LIF) was demonstrated as part of the Fernald Environmental Management Project (FEMP) Plant 1 Large Scale Demonstration and Deployment Project (LSDDP) sponsored by the U.S. DOE Office of Science and Technology, Deactivation and Decommissioning Focus Area located at the Federal Energy Technology Center (FETC) in Morgantown, WV. The demonstration took place on November 19, 1996. LIF works by using laser light to cause an excitation of the uranium oxide molecules that may be present as a surface contaminant. Energy is released from the molecules in the form of fluorescence that is then detected using a close-coupled device (CCD) camera (i.e., video camera) and displayed on a monitor attached to the laser. The LIF system consists of two major elements: the component comprised of both the laser cooling and laser control subsystems, and the tripod-mounted component consisting of the laser, CCD camera, and monitor.  
<http://apps.em.doe.gov/ost/itsrall.html>

#### Airborne Passive FT-IR Spectrometry

Kroutil, Robert T. (U.S. Army Edgewood Chemical Biological Center), R.J. Combs, R.B. Knapp; Gary W. Small (Ohio Univ.).

Vibrational Spectroscopy-based Sensor Systems. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4577, p 213-225, 2002

This project demonstrates the use of a commercially available passive Fourier transform infrared (FTIR) spectrometer to detect, identify, and quantify ammonia and ethanol vapor signatures based on the appropriate signal-processing strategy. The signal-processing strategy removes the need for a representative background spectrum through the use of three steps to extract the spectral information associated with the target vapor. The first step is optimal interferogram segment selection, which depends on the bandwidth of the target spectral feature. The second step applies the statistically significant finite impulse responses matrix filter to the optimal interferogram segment to attenuate spectral interferences. The third step quantifies the FIRM filter results with a discriminant analysis. Low-altitude airborne passive FTIR spectrometry allows rapid quantitative detection of plumes of ammonia and ethanol vapor. This work also documents the direct interferogram analysis of data from the fast scanning airborne passive FTIR spectrometer.

#### Ambient Formaldehyde Detection with a Laser Spectrometer Based on Difference-Frequency Generation in PPLN

Rehle, D. (Rice Univ., Houston, TX); D. Leleux; M. Erdelyi; F. Tittel; M. Fraser; S. Friedfeld.  
Applied Physics B: Lasers and Optics, Vol 72, 947-952, 2001

A laser spectrometer based on difference-frequency generation in periodically poled LiNbO<sub>3</sub> (PPLN) has been developed to quantify atmospheric formaldehyde with a detection limit of 0.32 ppb in a given volume (ppbV) using specifically developed data-processing techniques and state-of-the-art fiber-coupled diode-laser pump sources at 1083 nm and 1561 nm. The authors compare field monitoring spectroscopic data with results obtained by a well-established wet-chemical o-(2,3,4,5,6-pentafluorobenzyl) hydroxylamine (PFBHA) technique.

Annotated Bibliography of Geophysical Methods for Characterizing Mine Waste, Late-1994 Through Early-2000

Campbell, D.L.

U.S. Geological Survey Open-File Report 00-428, 12 pp, 2000

Abstract not available.

Application of Advanced Geophysical Logging Methods in the Characterization of a Fractured-Sedimentary Bedrock Aquifer, Ventura County, California

Williams, J.H.; J.W. Lane; K. Singha; F.P. Haeni.

U.S. Geological Survey Water-Resources Investigations Report 00-4083, 28 pp, 2002

An integrated suite of advanced geophysical logging methods was used to characterize the geology and hydrology of three boreholes completed in fractured-sedimentary bedrock in Ventura County, CA. The geophysical methods included caliper, gamma, electromagnetic induction, borehole deviation, optical and acoustic televiewer, borehole radar, fluid resistivity, temperature, and electromagnetic flowmeter. The geophysical logging provided insights useful for the overall geohydrologic characterization of the bedrock and enhanced the value of information collected by other methods from the boreholes, including core-sample analysis, multiple-level monitoring, and packer testing. The logged boreholes, which have open intervals of 100 to 200 feet, penetrate a sequence of interbedded sandstone and mudstone with bedding striking 220 to 250 degrees and dipping 15 to 40 degrees to the northwest. Fractures intersected by the boreholes include fractures parallel to bedding and fractures with variable strike that dip moderately to steeply. Two to three flow zones were detected in each borehole. The flow zones consist of bedding-parallel or steeply dipping fractures or a combination of bedding-parallel fractures and moderately to steeply dipping fractures. About 75 to more than 90% of the measured flow under pumped conditions was produced by only one of the flow zones in each borehole.

<http://ny.usgs.gov/pubs/wri/wri004083/>

Application of Multivariate Optical Computing to Simple Near-Infrared Point Measurements

Myrick, M.L. (Univ. of South Carolina); O.O. Soyemi; M.V. Schiza; J.R. Farr; F. Haibach; A. Greer; H. Li; R. Priore.

Instrumentation for Air Pollution and Global Atmospheric Monitoring. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4574, p 208-215, 2002

Quantitative multivariate spectroscopic methods need spectral patterns that correspond to analyte concentrations even in the presence of interferents. With the goal of producing a field-portable instrument, bulky and complex instrumentation can be eliminated by embedding a spectral pattern that corresponds to a target analyte in an interference filter in a beamsplitter arrangement. The authors evaluate a candidate filter design for an organic analyte and an interferent.

Applications of In-Water Mass Spectrometry for Detection of Volatile Organic Compounds and Dissolved Gases

Short, R.T. (Univ. of South Florida, Center for Ocean Technology); D.P. Fries; G. Kibelka; M.L. Kerr; S.K. Toler; P.G. Wenner; R.H. Byrne.

Second Workshop on Harsh-Environment Mass Spectrometry, 18-21 March 2001, St. Petersburg, Florida.

The authors have developed and deployed two underwater membrane introduction mass spectrometry (MIMS) systems that can operate autonomously or under user control via a wireless rf link. The initial

underwater MIMS systems uses a linear quadrupole mass filter, provides detection limits for most volatile organic compounds (VOCs) in the 1-5 ppb range, and has a power requirement of 95 Watts. In addition, the quadrupole MIMS system can be used for in situ dissolved gas analysis. The second version uses an ion trap mass spectrometer, provides detection limits below 1 ppb for most VOCs and consumes on the order of 150 Watts. Both systems can be deployed either as moored sensors or on unmanned underwater vehicles. Data have been collected from each of the two systems under a variety of deployment scenarios: the quadrupole system has been used to monitor wastewater influent (toluene and chloroform concentrations) over a period of several days; the system also has been used for in situ studies of hydrothermal vents in the Gulf of Mexico; the ion trap system has monitored gasoline exhaust from marina motor boat traffic to detect a VOC component (toluene); the researchers have also deployed the system on an autonomous guided underwater vehicle to investigate the integrated system utility for detection of chemical spills or plumes of other chemicals in the water column.  
<http://cot.marine.usf.edu/hems/workshop/2ndworkshop/Short/index.htm>

#### Array Biosensor for Environmental Monitoring

Ligler, F.S. (Naval Research Lab.); K.E. Sapsford (George Mason Univ.); Y.S. Shubin (Geo-Centers, Inc.); J. Lemmond (Hofstra Univ.); C.A. Rowe-Taitt (Naval Research Lab.), J.B. Delahanty, J.P. Golden.

Advanced Environmental Sensing Technology II. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4576, p 63-67, 2002

The automated, portable, array biosensor can detect and identify multiple analytes in multiple samples simultaneously using fluorescence immunoassays on a planar waveguide and miniaturized fluidics. Assays require 12 minutes to perform. False positive or false negative results due to environmental contaminants in the sample have not been seen. Measurements can be conducted in real time using spots as small as 80 micrometers.

#### Assessment of Inner Filter Effects in Fluorescence Spectroscopy Using the Dual-Pathlength Method: a Study of the Jet Fuel JP-4

Pagano, Todd E.; Jonathan E. Kenny, Tufts Univ.

Internal Standardization and Calibration Architectures for Chemical Sensors. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3856, p 289-297, 1999

This paper presents the photophysical background theory of inner filtering, with a comparison of existing correction schemes, and introduces the dual-pathlength method, a novel and simple experimental procedure for inner filter effect compensation. The authors evaluate the role of inner filtering in JP-4, a jet fuel contaminant detected by a laser-induced fluorescence/cone penetrometer instrument.

#### Automated Ground-Water Monitoring with Robowell: Case Studies and Potential Applications

Granato, Gregory E.; Kirk P. Smith, U.S. Geological Survey.

Chemical and Biological Early Warning Monitoring for Water, Food, and Ground. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4575, p 32-41, 2002

Robowell is an automated system and method for monitoring ground-water quality. The system can communicate data and system performance through a remote communication link. Six Robowell prototypes have successfully monitored ground-water quality during all four seasons of the year under different hydrogeologic conditions, well designs, and geochemical environments. The U.S. Geological Survey is seeking partners for research with robust and economical water-quality monitoring

instruments designed to measure contaminants of concern in conjunction with the application and commercialization of the Robowell technology. Project publications and information about technology transfer opportunities are available on the Internet.  
<http://ma.water.usgs.gov/automon/>

An Automatic Measurement of Hydrogen Cyanide in Air by a Monitoring Tape Method  
Nakano N.(Riken Keiki Co., Ltd., Tokyo, Japan), A. Yamamoto; Y Kobayashi (Kogakuin Univ. Tokyo, Japan), K. Nagashima.  
*Analytica Chimica Acta*, Vol 398 No 2-3, p 305-310, 1999

An automatic monitor has been developed for hydrogen cyanide gas in air using a sensitive tape for hydrogen cyanide. It is based on color change of the tape by reaction with hydrogen cyanide. The tape has been found to be a highly sensitive means of detecting hydrogen cyanide gas, and it maintained stable sensitivity for at least a month in the air of a desiccator. The detection limit (S/N=3) was 0.2ppm for hydrogen cyanide gas with a sampling time of 60s and a flow rate of 400ml/min. No response was observed from methanol (1vol.%), acetone (1vol.%), carbon dioxide (4.9vol.%), carbon monoxide (100ppm), sulfur dioxide (50ppm), hydrogen chloride gas (8ppm), nitrogen monoxide (50ppm), nitrogen dioxide (4ppm), or ammonia (40ppm).

Autorange Compensation for Variable Baseline Chemical Sensors  
McKnoch, Sam; Denise M. Wilson, Univ. of Washington.  
*Advanced Environmental Sensing Technology II. Proceedings of SPIE - The International Society for Optical Engineering*, Vol 4576, p 96-107, 2002

The authors present a generic circuit for auto-calibrating and compensating for the baseline of a variety of chemiresistive devices to improve concentration measurement resolution and analyte discrimination. The measurement circuits optimize sensor resolution via baseline compensation in the context of processing resistance changes from composite polymer chemical sensors and tin-oxide chemical sensors. Dynamic range is standardized to a constant size regardless of initial baseline resistances. The resulting dynamic range can be as much as two orders smaller than an uncompensated circuit and achieve the same sensor accuracy. Simulations have also shown a considerable improvement in resolution.

Biosensors Based on Bilayer Lipid Membranes for Automated Continuous Monitoring or Rapid Screening of Environmental Pollutants  
Nikolelis, Dimitrios P. (Univ. of Athens, Athens, Greece); Christina G. Siontorou; Vangelis G. Andreou. *Laboratory Robotics and Automation*, Vol 9, No 6, p 285-295, 1997

This paper describes applications of bilayer lipid membranes (BLMs) in the automated continuous monitoring or rapid screening (in a single format) of environmental pollutants, i.e., triazine herbicides (simazine, atrazine, and propazine). A continuous flow mode was used and injections of herbicides were made into flowing streams of a carrier electrolyte solution. A transient current signal (with a magnitude related to the herbicide concentration) reproducibly appeared in less than 2 minutes after exposure of the lipid membranes to the herbicides and increased in the order of simazine, atrazine, and propazine that allowed selective detection and analysis of these triazines in mixtures. The system is regenerable and can be used for repetitive cycles of injections. The minisensors have exhibited good mechanical stability and longevity (over 48 hours), and constant sensitivity and response to a given concentration of analyte in solution. The sensors can be easily and reliably fabricated at low cost and provide the advantages of fast response times (in the order of seconds) to alterations of analyte concentration, low

detection limits ( $\sim 10^{-6}$  M for ammonium ions and  $\sim 10^{-9}$  M for carbon dioxide, triazines, or cyanide ions), and the capability of analyzing small sample volumes.

BIOSET: Biosensors for Environmental Technology. State of the Art 2000

Alcock, S.J.; J.D. Newman (eds.).

European Union Concerted Action, 47 pp, Sep 2000

A European Union Concerted Action on 'Biosensors for environmental monitoring/environmental technology' (BIOSET) operated over the period 1997-2000. The aim was to guide technological developments in the field of biosensors for environmental monitoring. Its focus was on the enhancement of the development of biosensors for practical applications in monitoring environmental pollutants in water, soil, waste, and air. The work was based on a series of European meetings, a centralized information facility, and a broad collaboration program. The BIOSET network has been succeeded by the EU Thematic Network on 'Sensors for Monitoring Water Pollution from Contaminated Land, Landfills and Sediment' (SENSPOL at <http://www.cranfield.ac.uk/biotech/senspol.htm>).  
<http://www.cranfield.ac.uk/biotech/bioset.htm>

Calibration Systems for Surface Plasmon Resonance Spectroscopy

Boysworth, Marc K. (Arizona State Univ.); Louis A. Obando; Karl S. Booksh.

Internal Standardization and Calibration Architectures for Chemical Sensors. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3856, p 308-316, 1999

The authors describe the development of novel, field-portable, inexpensive, and easy-to-fabricate optical fiber waveguide surface plasmon resonance (SPR) sensors. These sensors generate SPR features that are broader than prism-based SPR features. Multivariate calibration has shown a 50% improvement in predictive accuracy compared to univariate methods. Traditional and new calibration methods for SPR are discussed, and recommendations are made regarding choice of regression modes, data density, and calibration set makeup.

A Case Study To Detect the Leakage of Underground Pressureless Cement Sewage Water Pipe Using GPR, Electrical, and Chemical Data

Liu, Guanqun; Yonggang Jia; Hongjun Liu; Hanxue Qiu; Dongling Qiu; Hongxian Shan.

Environmental Science & Technology, Volume 36 Number 5, p 1077-1085, 1 Mar 2002

This paper introduces a comprehensive method combining ground penetrating radar (GPR), electric potential survey, and geochemical survey for the detection of leakage in an underground pressureless nonmetallic sewage pipe. Verification of the method through subsequent excavation has shown that determining the suspected location by anomaly type is effective and economical.

Characterisation of the Phosgene Response of a Membrane Inlet  $^{63}\text{Ni}$  Ion Mobility Spectrometer

Bocos-Bintintan, Victor (Technical Univ. of Cluj-Napoca, Romania); Alan Brittain (Graseby Dynamics Ltd in Watford, UK); C.L. Paul Thomas (Univ. of Manchester, UK).

The Analyst, Vol 127 No 9, p 1211-1217, 2002

Ion mobility mass spectrometry has been developed as a monitoring technique for the toxic compound phosgene (carbonyl chloride, which smells of hay). The researchers hope the system will be developed as a viable monitoring system for the industrial workplace, in phosgene handling, storage, and transport. and in assessing military waste. Ion mobility spectrometry with a membrane inlet for the device can be coupled with a quadrupole mass spectrometer to produce consistent results for dry air samples

containing phosgene. The system is capable of detecting far less than the toxic limit of phosgene at just 1 milligram per cubic meter, with an upper limit of 32 mg m<sup>-3</sup>.

#### Characterization of Polymer-Coated QCRs in the Detection of Organic Compounds in Liquid Environments

Josse, Fabien J. (Marquette Univ.), R. Zhou, R. Patel, K. Zinszer; R.W. Cernosek (Sandia National Labs.).

Internal Standardization and Calibration Architectures for Chemical Sensors. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3856, p 109-118, 1999

The design of sensor arrays using polymer-coated QCRs for the practical detection of organic compounds in aqueous environments requires the appropriate selection of sensitive coatings, such as the rubbery and glassy polymers the authors investigated. The targeted analytes include classes of polar compounds, nonpolar compounds, and chlorinated hydrocarbons. Changes in viscoelastic properties during and after analyte sorption can be significant enough to place the sensor in the non-gravimetric regime, but for most applications involving relatively low concentrations of organic compounds, the subsequent change in viscoelastic properties are still such that the sensors operate in the linear regime, so the calculated partition coefficients can still be used for an approximate classification and selection of the coatings.

#### Chemical Cloud Tracking Systems

Grim, Larry B. (MESH, Inc.), T.C. Gruber; M. Marshall (U.S. Army, Dugway Proving Ground), B. Rowland.

Instrumentation for Air Pollution and Global Atmospheric Monitoring. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4574, p 1-6, 2002

A Chemical Cloud Tracking System (CCTS) has been installed at Dugway Proving Ground that allows mapping of chemical clouds in real time from a safe standoff distance. FTIRs perform passive standoff chemical agent detection. Each instrument individually can only measure the total of all the chemical in its line of site; the distance to the cloud is unknown. By merging data from multiple vantage points (either one instrument moving past the cloud or two or more instruments spaced so as to view the cloud from different directions), a map of the cloud locations can be generated using tomography. To improve the sensitivity and accuracy of the cloud map, chemical point sensors can be added to the sensor array being used. The equipment works on the move, which allows rapid response to emergency situations such as plant explosions, tanker car accidents, and chemical terrorism.

#### Chemical Imaging Cameras: the First Steps

Crocombe, Richard A. (Bio-Rad Labs), E.V. Miseo, N.A. Wright; K.J. Beltis (Arthur D. Little, Inc.), A.S. Louie.

Vibrational Spectroscopy-based Sensor Systems. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4577, p 89-94, 2002

This paper describes the use of a fast readout MCT focal plane array for spectrochemical imaging.

#### Chemical Imaging System

Jensen, James O. (U.S. Army Soldier and Biological Chemical Command), A.I. Ifarraguerri, W.R. Loerop; W. Wadsworth (Designs and Prototypes, Ltd.), J.-P. Dybwad.

Instrumentation for Air Pollution and Global Atmospheric Monitoring. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4574, p 52-62, 2002

The U.S. Army is developing a Chemical Imaging System (CIS), a small, high-speed, long-wave, infrared (8-12 micrometers) imaging spectrometer. The fielded system will operate at 360 scans per second with a large format focal-plane-array. Currently, the CIS uses the TurboFT FTS in conjunction with a 16-pixel direct-wired HgCdTe detector array. The TurboFT-based system requires a non-uniform sampling Fourier transform algorithm to preserve signal fidelity. Due to the enormous amount of data generated, signal processing must proceed at very high rate, so high-speed computers operating with a parallel architecture process the data in real time. This paper describes the current CIS breadbox system.

Chemical Sensing System for Classification of Minelike Objects by Explosives Detection  
Chambers, William B. (Sandia National Labs.); P.J. Rodacy; E.E. Jones; B.J. Gomez; R.L. Woodfin.  
Detection and Remediation Technologies for Mines and Minelike Targets III. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3392, p 453-461, 1998

Sandia National Laboratories has conducted research in chemical sensing and analysis of explosives that has focused recently on the classification of UXO in shallow water and anti-personnel/anti tank mines on land, and more specifically, on the development a field-portable chemical sensing system for examining mine-like objects to determine whether there are explosive molecules associated with them. Two sampling subsystems have been designed, one for water collection and one for soil/vapor sampling. The chemical sensing system is capable of sub-ppb detection of TNT and related explosive compounds. The paper presents the results of field and laboratory tests for the detection of buried explosives.

Chemical Sensing Using Infrared Flattened-Fiber Evanescent-Wave Spectroscopy  
Spector, Oded (Tel Aviv Univ.); A. German; L. Nagly; A. Katzir.  
Infrared Optical Fibers and Their Applications. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3849, p 189-195, 1999

This paper describes a technique for enhancing the signal of fiber-optic evanescent wave spectroscopy (FEWS) in the infrared region, by flattening the sensing part of the fiber. FEWS is a novel method for measuring the absorption spectra of chemicals in contact with a segment of an optical fiber. It enables remote in-situ measurements using an optically closed system. A technique for flattening a central part of silver-halide ( $\text{AgCl}_x\text{Br}_{1-x}$ ) fibers was developed that can produce fibers as small as 50 micrometers in thickness. The text includes the results of tests of sensor performance.

Chemical Sensors and Analyzers for In Situ Measurements in the Ocean: Long-Term, Autonomous Observations in Extreme Environments from the Antarctic to Deep-Sea Hydrothermal Vents  
Johnson, Kenneth S. (Monterey Bay Aquarium Research Inst.); L.J. Coletti; H.W. Jannasch; T.P. Chapin; C.M. Sakamoto.  
In Situ Instruments Workshop, 11-13 June 2002, Pasadena, California. NASA, Jet Propulsion Laboratory, Center for In-Situ Exploration and Sample Return.

The Chemical Sensor Laboratory at the Monterey Bay Aquarium Research Institute (MBARI) has developed a variety of chemical sensors and analyzers that are designed for in situ, autonomous observations. Measurements of redox-reactive inorganic nutrient chemicals such as nitrate, sulfide, iron, and manganese have been made for time periods up to one year without operator intervention. These instruments have been deployed throughout the ocean, in environments including deep-sea hydrothermal vents, the Southern Ocean, equatorial Pacific, coastal upwelling systems, and shallow



marine ponds to study the role of nutrients in regulating ecosystem processes. This paper involves a brief review of the instruments and deployments in some of the most challenging environments, as well as lessons learned.

#### Chemically Selective Coated Quartz-Crystal-Microbalance (QCM) Array for Detection of Volatile Organic Chemicals

Schneider, T.W. (Sandia National Labs.); G.C. Frye-Mason; S.J. Martin; J.J. Spates; T.V. Bohuszewicz; G.C. Osbourn; J.W. Bartholomew.

Chemical Microsensors and Applications. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3539, p 85-94, 1998

Liquid flow cells have been fabricated to prepare quartz-crystal-microbalance (QCM) arrays operating simultaneously for detection and identification of VOCs in water. Nine different polymer coatings applied using a spin coat technique have been examined for VOC response under liquid flow conditions. A matrix of three classes of VOCs (polar, nonpolar and chlorinated) were examined for each coating with four chemicals in each class.

#### Compact and Rugged Multipurpose TOF

Gonin, M. (Ionwerks, Inc., Houston, TX); K. Fuhrer; J.A. Schultz.

Second Workshop on Harsh-Environment Mass Spectrometry, 18-21 March 2001, St. Petersburg, Florida

The authors have developed for NASA a relatively compact (10" x 10" x 2.5") time-of-flight mass spectrometer for a wide range of applications, especially in harsh environments. The instrument has a resolving power of  $m/Dm = 800$  FWHM, and a sensitivity of 10 ppm in one second for the analysis of gases and existing ions (e.g., it can monitor gas composition and detect process failures within one second). A version with higher ion energies has been developed for very rapid sampling (90 kHz) and higher resolution ( $m/Dm = 1500$ ). The initial purpose of the instrument is the real-time monitoring of rocket exhausts during take off.

<http://cot.marine.usf.edu/hems/workshop/2ndworkshop/presentation.htm>

#### Comparison of Field- and Laboratory-Collected Midwave and Longwave Infrared Emissivity Spectra/Data Reduction Techniques

Salvaggio, Carl; Craig J. Miller, Spectral Information Technology Applications Ctr.

Algorithms for Multispectral, Hyperspectral, and Ultraspectral Imagery VII. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4381, p 549-558, 2001

The propagation of numerous devices for the measurement of midwave and longwave emissivity in the field has occurred in recent years. The researchers demonstrate temperature/emissivity separation algorithms on data collected with a field portable Fourier transform infrared (FTIR) spectrometer and compare the merits and resulting accuracy to laboratory spectra made of identical samples. Readers also are alerted to the possible sources of error in these spectra that may result when using sensing systems that do not look straight down on targets or when their nadir looking sensor is looking at a tilted target.

#### Comparison of Near and Mid-Infrared Tunable Diode Laser Absorption Spectroscopy for the Analysis of Combustion Gases

Miller, J.H., National Institute of Standards and Technology. Annual Conference on Fire Research: Book of Abstracts. November 2-5, 1998, Gaithersburg, MD. p 19-20, 1998

The need for reliable, rapid, and accurate measurements of species concentrations in flames has been the motivation for the development of laser diagnostics for more than 20 years. Scientists at NIST have used mid-infrared (defined here as 3.5 to 16  $\mu\text{m}$ ) diode lasers to characterize the concentration of carbon monoxide and local flame temperature in methane/air and ethylene/air diffusion flames supported on laboratory scale burners. TDLAS has also been used for the detection of methane, carbon dioxide, and acetylene in a laboratory burner designed to model upset conditions in a hazardous waste incinerator. A limitation of the mid-infrared diode laser technology is the requirement for cryoscopic temperatures for the laser's operation and the high cost of both the devices and the detectors required at these wavelengths. In contrast, visible- and near-infrared lasers (and detectors) are relatively cheap. Further, low-loss and inexpensive optical fibers do not exist for the longer wavelength devices and application of the technology to systems with limited optical accessibility is hampered. The Building and Fire Research Laboratory of NIST has obtained a near infrared system for the analysis of combustion gases and initiated a research program for the development of spectral simulation and fitting software for both the mid and near infrared, and a side-by-side comparison of mid- and near-infrared technologies for in situ analysis.

<http://fire.nist.gov/bfrlpubs/fire98/PDF/f98128.pdf>

Comparison of Passive Diffusion Bag Samplers and Submersible Pump Sampling Methods for Monitoring Volatile Organic Compounds in Ground Water at Area 6, Naval Air Station Whidbey Island, Washington

Huffman, Reagan L., U.S. Geological Survey, Tacoma, WA.

USGS Water-Resources Investigations Report 02-4203, 32 pp, 2002

Ground-water samples were collected in April 1999 at Naval Air Station Whidbey Island, WA, with passive diffusion samplers and a submersible pump to compare concentrations of volatile organic compounds (VOCs) in water samples collected using the two sampling methods. Single diffusion samplers were installed in wells with 10-foot screened intervals, and multiple diffusion samplers were installed in wells with 20- to 40-foot screened intervals. The diffusion samplers were recovered after 20 days and the wells were then sampled using a submersible pump. VOC concentrations in the 10-foot screened wells in water samples collected with diffusion samplers closely matched concentrations in samples collected with the submersible pump. Analysis of VOC concentrations in samples collected from the 20- to 40-foot screened wells with multiple diffusion samplers indicated vertical concentration variation within the screened interval, whereas the analysis of VOC concentrations in samples collected with the submersible pump indicated mixing during pumping. The results obtained using the two sampling methods indicate that the samples collected with the diffusion samplers were comparable with and can be considerably less expensive than samples collected using a submersible pump.

<http://water.usgs.gov/pubs/wri/wri024203/>

Complex Resistivity Tomography for Environmental Applications

Kemna, A.; A. Binley; A. Ramirez; W. Daily.

Chemical Engineering Journal, Vol 77 No 1-2, p 11-18, 2000

New tomographic methods are becoming available that will allow complex resistivity to be employed with arbitrary electrode arrangements. This paper reports laboratory trials of extensions of electrical resistivity tomography to a complex form. The inversion procedure is presented and demonstrated for a range of targets, with resistive and reactive characteristics.

Continuous Internal Response Calibration for FT-IR Spectrometry

Combs, Roger J. (U.S. Army Edgewood Chemical Biological Ctr.); C.J. Manning (Manning Applied Technologies, Inc.).

Vibrational Spectroscopy-Based Sensor Systems. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4577, p 135-147, 2002

Calibration of Fourier transform infrared (FTIR) spectrometer response is crucial to quantitative spectroradiometric measurements. The authors demonstrate the use of light emitting diodes (LEDs) as probes of detector channel response. LED modulation bandwidths, some extending well into the megaHertz (MHz) range, are more than fast enough for characterization of FTIR detector channel responses. A variety of optical probe signals can be generated using LEDs driven by waveform generators, lock-in amplifiers, or digital signal processors.

Controlled Emissions Demonstration Project Final Report—Gas Chromatograph/ Mass Spectrometry Mercury Monitor

MSE Technology Applications, Inc., Butte, MT.

Report No: PTP-74, 36 pp, Sep 2000

To address the mercury emission problems of U.S. DOE incinerators, MSE Technology Applications, Inc. (MSE), and the DOE Transuranic and Mixed Waste Focus Area are evaluating the feasibility of using gas chromatography (GC)/mass spectrometry (MS) for analyzing mercury and its compounds in the incineration offgases. The main objective of the program is to perform initial bench-scale testing to evaluate the most promising areas of development of the above-mentioned concept and report the advantages and disadvantages of the considered test configurations. From August 1999 to July 2000, MSE performed a literature search on mercury speciation analysis and tested analytical capabilities of the GC/electron-impact ionization (EI)/MS-based technique for analysis of mercury compounds. The experiments were carried out in the MS laboratory of the Chemistry Department at Montana State University—Bozeman. The intent of the experiments was to evaluate technical viability of the GC/EI/MS class instruments to analyze mercury species in the incineration offgases both qualitatively and quantitatively. The existing analytical methods can provide information on total and elemental mercury only and cannot distinguish the forms of speciated mercury. The performed tests demonstrated a possibility of mercury speciation analysis using GC/EI/MS equipment. Further development of the preconcentration techniques is required to obtain adequate detection limits for some of the mercury compounds, such as mercuric chloride.

<http://tmfa.inel.gov/Documents/technical.asp>

Controlled Emissions Demonstration Project—Pilot-Scale Testing Final Report for Accelerated Polychlorinated Dibenzo-P-Dioxins/ Dibenzofurans Sampling and Analysis (“Fast” Gas Chromatography/ Mass Spectrometry Dioxin/ Furan Analysis Method)

MSE Technology Applications, Inc., Butte, MT.

Report No: PTP-73, 54 pp, Sep 2000

The objective of the Accelerated Polychlorinated Dibenzo-p-dioxins/Dibenzofurans Sampling and Analysis (APSA) project (previously known at the “Fast” Gas Chromatography/Mass Spectrometry (GC/MS) Analysis Project) is to develop, test, and demonstrate an APSA system capable of on site sampling and analyses of dioxins/furans in incineration offgases with a turnaround time of as little as 2 hours. The APSA device is intended to be used for diagnostic (rather than compliance) monitoring; however, an advanced version may be suitable as a substitute for U.S. EPA Method 23. The APSA method being reported here is expected to be adaptable to nonthermal alternative treatment technology waste streams, either directly, for gaseous waste streams, or with minor modification for aqueous waste streams.

<http://tmfa.inel.gov/Documents/technical.asp>

### Copper Sensor System for Unattended Marine Operations II: Development of a Polymer Sensor and Field Tests

Lamontagne, Robert A. (Naval Research Lab.); J.W. Foerster (U.S. Naval Academy).

Internal Standardization and Calibration Architectures for Chemical Sensors. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3856, p 128-139, 1999

The copper-containing antifoulant coatings on ship hulls provide a major source of ionic copper (Cu(I) and (II)) trace metal contamination in the marine environment. Tracing this contamination is difficult because the ionic copper released from the coatings complexes rapidly with organic and inorganic ligands in the water column. This paper describes an examination of the potential for using the organic dye 2,9-dimethyl-4,7-diphenyl-1, 10-phenanthroine (BCP) embedded in the ionomeric polymer, Nafion 117, as a membrane probe sensor for quickly measuring ionic copper in seawater. Response times for these devices depend on the size of the membrane used. Presently, the optical comparator using a 2x3 membrane takes 20 minutes to develop color; a comparator has no electronic parts and requires only a comparison of color depth to determine the level of ionic copper in the sample. The fiber-optic probe uses a 0.5 cm diameter membrane that takes one minute.

### Cost and Performance Report for Tri-Service Site Characterization and Analysis Penetrometer System (SCAPS) Membrane Interface Probe

Myers, K.F. (U.S. Army Engineer Research and Development Center, Vicksburg, MS); W.M. Davis; J. Costanza. Report No: ERDC/EL TR-02-1, 42 pp, Jan 2002

Several demonstrations of the ion trap mass spectrometer-Membrane Interface Probe (ITMS-MIP) system for volatile organic compounds (VOCs) were completed between August of 1998 and May of 2000. The major emphasis of this report is the demonstration at NAS North Island in April-May 2000, which was specifically carried out as a production deployment. The ITMS-MIP system uses the commercially available MIP to collect vapor samples from the subsurface. The MIP collects VOC samples from the subsurface through a permeable membrane into a helium carrier gas that transports the sample above the ground surface for analysis. The analysis is performed in real time by a direct sampling ITMS in accordance with draft Method 8265 (USEPA, 1994). Approximately 4 minutes elapse from the time the MIP reaches the sample depth of interest until the analysis results are available. The production deployment at NAS North Island in April-May 2000 yielded 493 depth-discrete samples collected and analyzed from 28 different investigation locations. The complete characterization screening of the trichloroethene (TCE) plume required 15 days. The overall cost was \$112,556 for the collection and analysis of subsurface samples, cone penetrometer testing (CPT) soil classification, and the disposal of investigation-derived waste (IDW). A comparison between the actual costs from the April 2000 effort and the estimated cost of completing a similar effort with monitoring wells showed that using the ITMS-MIP system potentially saved \$38,000, a 25% cost saving. The ITMS-MIP produced 493 samples versus the 28 samples that would have been sampled and analyzed by installing and sampling conventional monitoring wells. The saving of cleanup time may be the greatest value added: the site managers are now at a decision point that they might not have reached for another two years if they had completed the characterization using conventional methods. The timesaving would not have been possible if the characterization had not been completed in one field deployment, which was made possible by the ability of the ITMS-MIP system to collect and analyze approximately 38 samples each day.

<http://www.wes.army.mil/el/elpubs/genrep.html>

Cyanide Determination: Problems Associated with the EPA/ASTM Approved Method for Determination of Total Cyanide  
Milosavljevic, E.B.; L. Solujic.  
Infomine, 1996

The EPA/ASTM approved method for determination of total cyanide is based on liberating HCN from a sample acidified with the sulfuric acid using an hour long reflux distillation procedure. The HCN gas formed is trapped by passing it through the high pH alkaline scrubbing solution. Cyanide concentration in this solution is then quantified by the spectrophotometric or potentiometric procedure. The total cyanide determination method often produces unreliable data. The method has low reproducibility and repeatability and serious interferences even from many ubiquitous species. The problems associated with the approved methods for cyanide determination has prompted EPA to look for solutions provided by different analytical methods, such as the agency-initiated validation study of EPA Method 1677 (Weak Acid Dissociable Cyanide by Ligand Exchange/Flow Injection/Amperometric Technique). The method tested is based on a recent study and has significant advantages over the EPA/ASTM approved procedures.

<http://www.infomine.com/technology/labmine/resources/cyanide.asp>

Data analysis Strategies for Passive Multispectral and Hyperspectral Infrared Remote Sensors  
Small, Gary W.; Lin Zhang, Ohio Univ.  
Vibrational Spectroscopy-based Sensor Systems.  
Proceedings of SPIE - The International Society for Optical Engineering, Vol 4577, p 115-126, 2002

The research presented in this paper describes the development of novel signal processing and pattern recognition methodology for application to multispectral imaging data and to non-imaging data acquired with a hyperspectral instrument. Remote sensing data were collected with these instruments mounted on an aircraft platform. The authors use data acquired at an industrial site to demonstrate the characteristics of each sensor and the data analysis methodology.

Design, Construction and Field Demonstration of Explorer: a Long-Range Untethered Live Gasline Inspection Robot System. Semi-Annual Report  
Vradis, George C. (New York Gas Group); Hagen Schempf (Robotics Inst., Carnegie Mellon Univ.).  
Report No: FC26-01NT41155-01, 23 pp, May 2002

The goal of this program is to construct and demonstrate EXPLORER, a modular, remotely controllable, self-powered, untethered robot system for the inspection of live gas distribution 150 mm (6-inch) to 200 mm (8-inch) diameter mains. The system, which was designed in an earlier effort, is built in a modular fashion to accommodate various components intended to accomplish different inspection, repair, sample retrieval, and other in-pipe tasks. The prototype system to be built under this project will include all the basic modules needed by the system, i.e., locomotion, power storage, wireless communication, and camera. The camera, a solid-state fisheye-type, is used to transmit real-time video to the operator that allows for the live inspection of gas distribution pipes. This module, which incorporates technology developed by NASA, has been designed, constructed and tested in the earlier effort. In the current effort, the full prototype system will be tested in the laboratory, followed by two field demonstrations in real applications in NYGAS member utilities' pipes. The purpose for EXPLORER is to be able to access live gas mains, insert the system in the piping network, and remotely 'drive' it within the gas main and its laterals through distances of five to ten thousand feet. Its adaptable locomotion system allows the robot to function through varying diameter pipes (150 - 200 mm or 6- to 8- inches) and is powered via on-board battery banks. The presence of fish-eye cameras in both ends of the robot allows the operator to view the forward and circumferential views of the internals live using

an above-ground TV. Communication takes place via wireless link between the robot and the launch-chamber used to insert/retrieve the system. This link is based on commercial technology presently employed in wireless telecommunication networks. Communication over long distances as well as battery re-charging will be accomplished without retrieving the robot through the use of auxiliaries, to be developed in a follow-on phase, that will allow insertion of additional antennas and battery recharge plugs into the pipe under live conditions through inexpensive keyhole-size excavations. The fabrication of the prototype should be completed by late summer 2002. Testing of the prototype in the lab is expected to be completed by November 2002, to be followed by two field demonstrations in early 2003.

[http://www.osti.gov/bridge/product.biblio.jsp?osti\\_id=801215](http://www.osti.gov/bridge/product.biblio.jsp?osti_id=801215)

#### Design of an Automated Rapid Vapor Concentrator and its Application in Nitroaromatic Vapor Sampling

Gehrke, Mark; S. Kapila; K.L. Hambacker; V.I. Flanigan, Univ. of Missouri, Rolla.

Detection and Remediation Technologies for Mines and Minelike Targets V. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4038, p 1352-1363, 2000

An automated, rapid-cycling vapor concentrator and sample introduction device was designed and evaluated. The device consists of an inert deactivated fused silica capillary sampling loop. The temperature of the loop was manipulated through contact with a cold plate or a hot plate, maintained at pre-selected temperatures with a thermoelectric cooler and heating cartridge, respectively. The position of the loop was controlled with a stepper motor under microprocessor control. The low mass of the loop permit its rapid cooling and heating with efficient trapping of adsorptive vapors such as nitroaromatics from the air stream, plus rapid and quantitative transfer of the trapped analytes to the detection system. The thermoelectric cooler supports variable trapping temperatures and increased sampling selectivity without the use of cryogenic fluids. Chemically inert sampling train surfaces prevent analyte loss due to irreversible adsorption and cross contamination between samples. Coupled with a selective electron capture detection system, the device was evaluated for rapid analysis of nitroaromatic and chlorinated aromatic vapors from air streams at trace concentrations. Trapping efficiencies of >95 percent were obtained with the device for nitroaromatics at ppb and sub-ppb concentrations.

#### Detection and Mapping of Fractures and Cavities Using Borehole Radar

Haeni, F.P. (Geophysical Consulting); Lucien Halleux (G-Tec); Carole D. Johnson (U.S. Geological Survey) and John W. Lane, Jr.

Proceedings: Fractured Rock 2002, 13-15 March 2002, Denver, Colorado. National Ground Water Association, Westerville, OH, 4pp.

Borehole radar can be used in a single-hole reflection mode or in a cross-hole tomography mode. In the reflection mode, radar provides an image of discontinuities in the bedrock surrounding a borehole, including bedding planes, lithologic contacts, fractures, and cavities. The measurements are either directional or omni-directional, depending upon the type of equipment and antennas. In the tomography mode, where the transmitter and receiver are in separate boreholes, radar provides an image of the planar section between the boreholes. The radius of investigation depends on the antenna frequency and the electrical conductivity of the bedrock. For a central frequency of 100 megahertz, in the reflection mode the ranges are typically 10 to 40 meters in resistive solid rock and less than 5 meters in conductive, clay-rich, or silty rock. Single-hole and cross-hole radar also have been used for water-supply investigations in the northeastern United States. Borehole radar was used to investigate crystalline bedrock in two rapidly developing communities that rely on water resources in the bedrock. The surveys were conducted and interpreted along with data from other borehole geophysical tools. The borehole radar surveys were used to identify the location and orientation of reflectors, locate the

primary pathways of flow to the supply wells, and identify aquifer characteristics that may be useful in siting a production well and protecting high-yielding wells in crystalline rocks. Borehole radar has been used to investigate fractures, cavities, and lithologic changes at several sites in Europe. The radar data has been interpreted in conjunction with the results of modeling of borehole-radar response. At the Grimsel nuclear waste laboratory in Switzerland, single-hole reflection and tomography methods were used to characterize the rock in inclined boreholes. At numerous geotechnical sites in Belgium, France, and the Netherlands, borehole radar has been used to characterize the rock and identify fractures and cavities.

[http://water.usgs.gov/ogw/bgas/publications/FracRock02\\_haeni/](http://water.usgs.gov/ogw/bgas/publications/FracRock02_haeni/)

Detection of Chemical Agents in the Atmosphere by Passive IR Remote Sensing

Beil, Andreas (Bruker Saxonika Analytik GmbH), R. Baum; T.J. Johnson (Bruker Optics).

Internal Standardization and Calibration Architectures for Chemical Sensors. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3856, p 44-56, 1999

Field releases of ammonia were identified with passive FTIR remote sensing from several observation points at 600 m, 1.5 km and 2.4 km. The results clearly demonstrate that reliable IR remote sensing of hazardous chemical agents in the atmosphere is possible with a highly sensitive instrument, an optimized measurement technique, and a sophisticated evaluation software.

Detection of Microorganisms with MS: Field-Portable Instrumentation and Innovative Methodology

Basile, F. (Colorado School of Mines), A. Madonna, K.J. Voorhees; S. Lammert (Oak Ridge National Lab); B. Musselman, V. Doroshenko (Science & Engineering Services, Inc.).

The 3rd Harsh-Environment Mass Spectrometry Workshop, 25-28 March 2002, Pasadena, California.

Research efforts over the last 17 years have contributed to the development of the Chemical Biological Mass Spectrometer (CBMS) for the U.S. Army. The CBMS detector is a field-portable MS system based on a quadrupole ion-trap mass analyzer and a sample pre-processing unit. The entire unit is about 5.8 cubic feet, 170 lbs, and operates at 24 Vdc at less than 500 W. The sample pre-processing unit consists of a high efficiency impactor (optimized for 2-10 mm particles) and a thermal reaction chamber. Collected microorganisms from bioaerosols are enriched in this chamber and thermally hydrolyzed and methylated to produce specific biomarker molecules, a process that takes place in under 10 seconds. Subsequent mass analysis of these molecules produces biomarker fingerprints that are characteristic to that microorganism. A more detailed description of the sample pre-processing step as well as the ion trap MS hardware will be presented for the latest version of the CBMS block II system. In addition, new directions and approaches in biodetection with MALDI-MS will be presented. Briefly, affinity separation techniques are coupled with MALDI-MS analysis for the detection of bacteria in complex environmental/biological mixtures. Examples will be shown where these new methodologies are coupled with an atmospheric-pressure MALDI-MS instrument in order to simplify future hardware designs for field-portable systems.

<http://cot.marine.usf.edu/hems/workshop/3rdworkshop/program.htm>

Detection of Soil Surface Contaminants by Infrared Reflection Spectroscopy

Blake, Thomas A.; Paul L. Gassman, Pacific Northwest National Lab.

Vibrational Spectroscopy-based Sensor Systems. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4577, p 239-261, 2002

A benchtop Fourier transform infrared spectrometer and specular reflection accessory have been used to record reflection spectra of chemical compounds (dimethyl methylphosphonate, trimethyl phosphate,

methylphosphonic acid, 2,2,6-thiodiethanol, diazinon, diesel fuel, and ammonium nitrate) coating a loamy, psamment soil. The soil reflection spectra have been compared to liquid or solid transmission spectra of the pure compound and frequency shifts with attention to relative intensity changes for the absorption features.

#### Detection of 'Unknown Agents' in Harsh Environments using a Newly Developed Ruggedized Mass Spectrometer

Hart, K.J. (Oak Ridge National Laboratory); I.F. Robbins; M.B. Wise; W.H. Griest; S.A. Lammert; C.V. Thompson.

The 3rd Harsh-Environment Mass Spectrometry Workshop, 25-28 March 2002 Pasadena, California.

A ruggedized and integrated detection system for chemical and biological agents has been developed for use in field analysis. The analyzer employed in this instrument is a custom designed ion trap mass spectrometer capable of using air as the buffer gas with complete electronic control and off-line data analysis software. System components have been selected for radiation tolerance and special circumvention circuits were designed to rapidly de-power the system upon detection of a nuclear event. The vacuum system includes a turbo pump tested to ensure it could operate without failure when exposed to vibrations and sudden changes in orientation that might be generated by the target vehicle platforms. The additional pumping speed obtained using this pumping strategy not only permits the system to clear itself more quickly than previous systems that were based on ion getter pumps but also allows the system to use chemical ionization reagents to increase chemical selectivity. The instrument is equipped with a mode-select valve to provide rapid selection of one of three sampling systems: a vapor detection line for volatile chemical agents, a ground sampling system for liquid chemical agents, and a unique aerosol concentrator/pyrolysis system for biological agents. The primary focus of this work has been the development of highly specific and reliable detection schemes for the most likely threat agents. This presentation discusses the instrument's application to the problem of detection of "unknown" chemical agents in harsh environments.

<http://cot.marine.usf.edu/hems/workshop/3rdworkshop/program.htm>

#### Determination of Cyanide in Waste Water by Low-Resolution Surface Enhanced Raman Spectroscopy on Sol-Gel Substrates

Premasiri, W. R. (Boston Univ., Boston, MA); R.H. Clarke; S. Londhe; M.E. Womble.

Journal of Raman Spectroscopy, Vol 32 No 11, p 919-922, Nov 2001

The authors introduce the concept of low-resolution surface enhanced Raman spectroscopy (SERS) for cyanide as a potentially highly useful, cost-effective approach to detection and analysis for monitoring water contamination. High-sensitivity, low-resolution measurements of cyanide in water can be made using a solid-state gold sol-gel substrate. The test data suggest a sensitivity limit for low-resolution SERS detection of cyanide in water in the region of 10 ppb.

#### Development and Validation of a Multisensor System for Ocean Pollution Detection

Navas, Ignasi (Univ. Politecnica de Catalunya), M. Bara, P. Prats, A. Broquetas; S. Charron (Thales Airborne Systems); F. Cabioch (CEDRE), R. Jezequel.

Remote Sensing for Environmental Monitoring, GIS Applications, and Geology. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4545, p 137-144, 2002

RAPSODI is a European project for the development of a new anti-pollution remote sensing system that results from the integration of airborne sensors: SAR, SLAR, IR, UV, a microwave radiometer, and spaceborne data. In a real size experiment in a completely controlled situation and environment, the



researchers released and treated heavy fuel oil. Another experiment involved monitoring the efficiency of the dispersing products used by the oil spill response community. This paper describes the development of the airborne SAR mode optimized for oil spill detection and the results of early experiments.

#### Development of a Low Cost Miniature Mass Spectrometer

Rohrs, H.W. (Mass Sensors, Inc., St. Louis, MO); W.R. Gentry; R.S. Chhatwal; P.S. Berger. Second Workshop on Harsh-Environment Mass Spectrometry, 18-21 March 2001, St. Petersburg, Florida.

The researchers' goal is to use new design and manufacturing technology to reduce the cost and size of MS solutions such that the units become portable and disposable. A 200-amu unit has been built based on a design pioneered by Diaz, Gentry, and Giese and licensed from the University of Minnesota. The first commercial prototype, an 80-amu unit is due for test in mid-April. The goal for both of these units is to reduce the cost of the core package (source, analyzer, and detector) to around \$500. This target would make the units disposable or recyclable and thus eliminate troubleshooting in favor of replacement. An embedded controller will deliver data over any Internet-based infrastructure, wired or wireless, with a browser-based user interface. A user with Internet access will be able to communicate with a network of remotely deployed sensors from anywhere at any time.

<http://cot.marine.usf.edu/hems/workshop/2ndworkshop/Rohrs/index.htm>

#### Development of a Technique for the Analysis of Inorganic Mercury Salts in Soils by Gas Chromatography/Mass Spectrometry

Barshick, C.M. (Oak Ridge National Lab., Oak Ridge, TN); S.-A. Barshick; P.F. Britt; D.A. Lake; M.A. Vance; E.B. Walsh.

International Journal of Mass Spectrometry, Vol 178 No 1-2, p 31-41, 1998

In a technique developed to analyze environmentally relevant samples for organic and inorganic mercury compounds, a solid-phase microextraction (SPME) fiber was used as a sampling medium in both water and water/soil slurries. The method quantifies inorganic mercury through a chemical alkylation reaction designed to convert an inorganic mercury salt to an organomercury compound prior to GC/MS analysis; this is the rate-limiting step in the analysis.

Methylbis(dimethylglyoximate)pyridinecobalt (III) was found to be a superior alkylating reagent because it produced a single reaction product, methylmercury iodide, with an efficiency of ~95%. Detection limits were ~7 ppb in water and ~2 ppm in soil.

#### Development of an In Situ Instrument for Measuring Mercury in a Gas Stream

Laudal, Dennis L., National Energy Technology Lab., Pittsburgh, PA.

Report No: FC21-94MC31388-40, 17 pp, Dec 2001

Sensor Research and Development Corporation (SRD) was contracted by DOE's National Energy Technology Laboratory (formerly the Federal Energy Technology Center) to develop a prototype instrument for thermal treatment process continuous emission monitoring applications. The SRD process has the potential to be the basis for a very low-cost mercury CEM. The initial cost estimates provided by SRD are an order of magnitude lower than any other proposed mercury CEM. Although the instrument will be low-cost, it still has the potential to detect low limits of mercury and so has a wide range of possible uses. In addition, the instrument will be very portable.

[http://www.osti.gov/bridge/product.biblio.jsp?osti\\_id=791043](http://www.osti.gov/bridge/product.biblio.jsp?osti_id=791043)

### Development of an Underwater Mass Spectrometer for Dissolved Gases, Solutes, and Large Organic Compounds

McMurtry, G.M. (SOEST, Univ. of Hawaii, Honolulu); Steven J. Smith (Jet Propulsion Lab./CalTech, Pasadena, CA).

Second Workshop on Harsh-Environment Mass Spectrometry, 18-21 March 2001, St. Petersburg, Florida.

The researchers are testing a shallow and deep-water mass spectrometer consisting of an aquatic-based sensor head, vacuum system pressure case, and associated electronics (called Mass SURFER). The entire unit fits within a 6.5-inch ID pressure vessel, 68 inches long, and incorporates the Rotating Field Mass Spectrometer (RFMS) developed at JPL. Seawater samples are admitted through one of three different introduction systems. The first is an osmotic membrane boundary and gas-based ionizer. The gas-sampler incorporates a hydrophobic membrane that has been successfully used in the lab to 200 bars hydrostatic pressure and in field deployments to 1300 meters water depth. The second interface is an on-line capillary nano-electrospray interface (ESI) nozzle capable of high-sensitivity mass spectrometry at nanoliter-per-minute flow rates. The seawater liquid with its load of dissolved gases is directly injected into submersible vacuum chamber. The challenge for this type of interface is clogging by fine suspended particles (course particles can be screened) and salts build-up. Direct seawater injections have produced no significant deleterious effects, but a small dialysis-like tip can be incorporated that is capable of salt removal approaching 100% for very low flow rates. The remaining water plus heavy organics are efficiently injected into the nanospray, which provides a direct liquid/vacuum interface. The third interface system includes a miniature capillary electrophoresis column that can presort large organic materials. Vacuum levels need only be at the millitorr level for a quality measurement, and the complete system nominally draws <10 watts. The RFMS mass resolution of 1 part in 500 is comparable with the best of other small mass spectrometers and it has extremely large analytical mass range (from 1 to >100,000 amu), making it capable of analyzing proteins and DNA fragments. The presentation includes recent spectra of seawater and large organic compounds, as well as the current development and field deployment status.

<http://cot.marine.usf.edu/hems/workshop/2ndworkshop/presentation.htm>

### Development of Eco-Sensor for the Continuous Monitoring of Environmental Volatile Organic Chlorinated Compounds

Murahashi, Mizuho (Japan Advanced Inst. of Science and Technology); Y. Ishimori (Toshiba Corp.), K. Kawano; T. Kase (Shimizu Corp.), M. Mouri; Y. Morita (Japan Advanced Inst. of Science and Technology), Y. Murakami, K. Yokoyama, E. Tamiya.

Advanced Environmental Sensing Technology II.

Proceedings of SPIE - The International Society for Optical Engineering, Vol 4576, p 255-262, 2002

The researchers have developed an advanced environmental monitoring system (AEMS) containing a sensor for the measurement of environmental pollutants. The eco-sensor is based on lipid membranes for continuous monitoring of underground water in industrial areas. The project has included the development of an automatic bilayer lipid membrane (BLM) preparation device. Eco-sensor sensitivity to volatile organic chlorinated compounds such as cis-1,2-dichloroethylene is in the order of 10 ppb using the monoolein BLMs in actual ground water. The next step will be to reduce the size of the eco-sensor for practical use. In addition to developing the sensor, the AEMS project is working to predict plume propagation using a computer simulation technique.

## Development of Neutron Probes for Characterization of Hazardous Materials in the Sub-Surface Medium

Keegan, R.P.; C.A. McGrath; J.C. Lopez, Idaho National Engineering and Environmental Laboratory, Idaho Falls, ID. Conference Paper No: INEEL/CON-02-00137, May 2002

Neutron probes are being developed at the Idaho National Engineering and Environmental Laboratory (INEEL) for the detection, identification and quantification of hazardous materials (e.g., plutonium, uranium, americium, chlorine, and fluorine) in the ground. Both a Neutron Gamma (NG) probe and a Prompt Fission Neutron (PFN) probe are being developed. The NG probe is used primarily for nuclide identification and quantification measurements. The PFN is used mostly for the detection and measurement of fissile material, but also for the determination of thermal neutron macroscopic absorption cross sections of the various elements comprising the ground matrix. Calibration of these probes will be carried out at the INEEL in an indoor facility designed for this activity.  
[http://www.osti.gov/bridge/product.biblio.jsp?osti\\_id=797105](http://www.osti.gov/bridge/product.biblio.jsp?osti_id=797105)

## Differential Helmholtz Resonator as an Photoacoustic Trace Gas Detector With Near-Infrared Diode Lasers

Kapitanov, V.A.; V. Zeninari; D. Courtois; Yu. N. Ponomarev, Groupe de Spectrometrie Moleculaire et Atmospherique, UPRES A CNRS, Reims Cedex 2, France; Laboratory of Atmospheric Absorption Spectroscopy, Inst. of Atmospheric Optics of SB RAS, Tomsk, Russia.  
TDLS 98: 2nd International Conference on Tunable Diode Laser Spectroscopy, 6-10 July 1998, Moscow, Russia. Book of Abstracts, p 20, 1998

The Helmholtz resonator (HR) for air pollution monitoring is simple in design and consists of two cell volumes connected together by a thin capillary. Compared to other resonators, the Helmholtz arrangement has the advantages of using cells of small volumes with low resonance frequency and the possibility to enhance the S/N ratio using differential schemes. The differential Helmholtz resonator (DHR) allows the user to double the signal amplitude and to minimize ambient noise. The double differential Helmholtz resonator (DDHR) additionally eliminates the most important part of the noise, the background signal. The research discussed here includes experimental study of HR and DHR responsiveness as applied to the detection of trace gases, and predictions of the responsiveness as a function of frequency, cell pressure, and cell design. The authors present simple Helmholtz resonator configuration for flow measurements and simple arrangement to enhance the main photoacoustic signal of the whole system by a factor of about 2.

## A Diode Laser/Cavity-Absorption Gas Sensor

Miller, J. Houston; Andrew R. Awtry, George Washington Univ.  
In Situ Instruments Workshop, 11-13 June 2002, Pasadena, California: Abstracts. NASA, Jet Propulsion Laboratory, Center for In-Situ Exploration and Sample Return.

The authors report their progress on the development of tunable diode laser gas sensor. A 1.55- $\mu\text{m}$  source has been incorporated in cw-Cavity Ringdown Spectroscopy (cw-CRDS), exploiting the sensitivity enhancement provided by the long effective sample path length of an optical cavity created between two mirrors. The current work has incorporated commercial off-the-shelf technologies from the telecommunications industry. Extension of this sensor platform technique to other wavelength regions in the near and mid infrared will increase the suite of molecules with accessible transitions. Results for carbon monoxide, carbon dioxide, ammonia, and hydrogen cyanide are presented as examples of sensitivity and detectivity; sensitivity levels of 10 ppb have been demonstrated for HCN.

#### E-Tongue 2 REDOX Response to Heavy Metals

Buehler, Martin G. (Jet Propulsion Laboratory), Gregory M. Kuhlman; Samuel P. Kounaves (Tufts Univ.).

In Situ Instruments Workshop, 11-13 June 2002, Pasadena, California: Abstracts. NASA, Jet Propulsion Laboratory, Center for In-Situ Exploration and Sample Return.

E-Tongue 2 is an array of electrochemical sensors including REDOX electrodes for CV (cyclic voltammetry) and ASV (anodic stripping voltammetry) measurements, Galvanic cells for corrosion measurements, and Ion Selective Electrodes. This paper presents recent results obtained from the REDOX electrodes used to detect Zn, Fe, and Cu in solution. The sensor utilizes a new electrode type produced by hybrid microelectronic techniques where metal electrodes are co-fired into ceramic substrates at 900 degrees C. This process produces very robust electrodes that can be mounted on the periphery of subsurface explorers to measure the electrochemistry of soils. Initial results from REDOX electrodes indicate response peaks are extremely sharply defined (half-width ~5 mV), and detection sensitivities are below 1  $\mu$ M for Cu. Determining the optimum detection conditions is discussed, where the supporting electrolyte (KCl) and ASV sweep rate (V/s) are varied over two orders of magnitude, while keeping the deposition time,  $T_{dep}$ , and analyte concentration constant. The methodology has been shown to have nM and sometimes pM sensitivities for the detection of metals in solution.

#### Enhanced Selectivity of Electron Capture Detector for Nitroaromatic Explosives Through the Application of Electron Attachment Reactions

Gehrke, Mark (Univ. of Missouri, Rolla); S. Kapila; V.I. Flanigan.

Detection and Remediation Technologies for Mines and Minelike Targets V.

Proceedings of SPIE - The International Society for Optical Engineering, Vol 4038, p 539-546, 2000

The researchers used the differences between the electron attachment reactions of thermal electrons and representative classes of organic molecules with high electron affinities selectively identify nitroaromatics, which showed that the reactions of thermal electrons with nitroaromatics lead to the formation of products with very low electron affinities. By contrast, other analytes with high electron affinities such as polyhalogenated organics, lead to products with high electron affinities. The researchers exploited this difference to differentiate between nitroaromatics and polychlorinated organics with a monitoring device—a tandem arrangement of two electron capture detectors connected in series with an electron attachment reactor. The tandem ECD arrangement provided selective determination of nitroaromatics vapors in the presence of interfering compounds at ppb and sub-ppb concentrations.

#### Enhancement in the Sensitivity of a Gas Biosensor by Using an Advanced Immobilization of a Recombinant Bioluminescent Bacterium

Gil, Geun Cheol; Young Joon Kim; Man Bock Gu, Kwang-Ju Inst. of Science and Technology (K-JIST), Puk-gu, Kwang-Ju, South Korea.

Biosensors and Bioelectronics, Vol 17 No 5, p 427-432, May 2002

A genetically engineered bioluminescent bacterium (*lac::luxCDABE*) was immobilized to develop a whole-cell biosensor for the detection of toxic gaseous chemicals. The bioluminescent reaction reduces in intensity when the cells experience toxic or lethal conditions. This whole-cell biosensor was fabricated with an immobilization technique on solid agar medium to measure toxicity through direct contact of the cells with a gas. The bioluminescent response is measured through a fiber optic probe connection between the biosensor kit and a luminometer. The biosensor has been tested on benzene, toluene, ethylbenzene, and xylenes (BTEX) vapors.

Electrochemical Detection for Gaseous Vinyl Chloride with a Sputtered Au/Porous Alumina Substrate/Pt Electrode Assembly

Chuang, Min-Chieh; Ming-Chang Yang, National Cheng Kung Univ., Tainan, Taiwan, ROC. Electroanalysis, Vol 14 No 17, p 1209-1214, Sep 2002

A detector with a porous alumina substrate has been developed to monitor vinyl chloride gas in the concentration range of 0.5-4% at room temperature. Higher sensitivities were obtained with tetrabutylammonium perchlorate as the supporting electrolyte than with tetrabutylammonium tetrafluoroborate, with the highest sensitivity of 70.9 A%<sup>-1</sup> obtained at -2.1 V (vs. Ag/Ag<sup>+</sup>) in 50% toluene/50% DMF electrolyte. The sensing current and the sensitivity for vinyl chloride increased significantly with the porosity of the porous alumina substrate.

Electrophoretic Repair of Impoundment Leaks: Analysis and Verification with Experimental Data  
Corapcioglu, M.Y.; K.K.R. Kambham; K. Tuncay, Texas A&M University, College Station, TX. Environmental Science & Technology, Vol 32 No 23, p 3778 -3784, 1998

A technique utilizing electrophoresis causes clay particles to be attracted toward leaks when an electric field is applied, providing cost-effective repair. This paper presents an experimentally verified means to predict electrophoretic sealing of in-service geomembrane liners, i.e., a procedure to simulate axis-symmetric electrophoretic cake formation and a numerical technique to solve the electric field for voltage gradients. In general, a higher voltage difference or a wider surface electrode accelerates the cake formation process. For efficient cake formation, the surface electrode should be located close to the water surface over the leak.

Environmental Geophysics to Delineate the 3-D Extent of DEEP chloride plumes at a Decommissioned Brine Pond near Hughenden, Alberta

Clarke, S.T.; L.M. Dumond, Essis Ltd., Calgary, Alberta

Remediation Technologies Symposium 2002, 16-18 October 2002, Banff, Alberta, Canada

Elevated chlorides discovered in ground-water wells were attributed to a brine pond resulting from washout disposal in salt caverns at Alkali Lake. A geophysical survey commenced in the winter of 2002 to delineate lateral and vertical extents of possible chloride plumes from Alkali Lake using the Geonics EM34 (EM induction) to determine the lateral extent of chloride-affected soils, which were alkaline and highly conductive. The direct-push Geoprobe SC400 (Wenner-Array AC injection) determined the vertical extent of EM-identified targets to depths of approximately 30 meters. An area approximately 14 km x 2 km was surveyed with the EM34 at 200 meter line spacing. Lateral closure was achieved on all anomalous trends, enabling the differentiation of naturally saline trends from possible chloride plumes. Two vertical conductivity profiles were targeted across possible chloride plumes. Anomalous conductivities were identified at ~30 meters in depth, yielding response magnitudes typical of very high chloride concentrations. Geoprobe cores helped differentiate between chloride-affected and naturally alkaline soils.

<http://www.remtech2002.com/agenda.htm>

Environmental Isotopes and Artificial Tracer Techniques for Investigation and Monitoring of Heterogeneous Aquifers

Tazioli, Alberto; Giulio Sergio Tazioli, Ancona Univ., Italy.

Investigacion, Gestion y Recuperacion de Acuiferos Contaminados, Oct 2001, Alicante, Spain.

Inst. of Geology and Mineralogy of Spain, Ministry of Science and Technology, Madrid, Spain.  
p 73-84, 2001

The paper presents the results of studies in Italy of artificial tracers and of geochemical and isotope analysis carried out in an alluvial plain polluted by Cr-VI from an industrial plant, and in three monitored sanitary landfills located in another upper alluvial plain. The values of the local background pollution parameters have allowed the interference of the landfill with the surface environment to be verified. The method utilized to control the interference of the landfill with underground environment, on defined hydrogeological situations, concerned a chemical and isotope control on surface water, groundwater, leachate and biogas. By application of artificial tracers, it was possible to determine the transfer time of pollution to ground water. [This is one of 11 papers in English out of 36 papers delivered at a Spanish-language conference.]

[http://www.igme.es/internet/web\\_aguas/igme/publica/lib15.htm](http://www.igme.es/internet/web_aguas/igme/publica/lib15.htm)

Environmental Technology Verification Report: Field Portable X-Ray Fluorescence Analyzer. HNU Systems SEFA-P. Superfund Innovative Technology Evaluation

Hess, E.; P. Splichal, PRC Environmental Management, Inc., Lenexa, KS, for the U.S. EPA, Las Vegas, NV. National Exposure Research Lab.

Report No: EPA/600/R-97/144; NTIS: PB2001-101679. 92 pp, Mar 1998

In April 1995, the U.S. EPA conducted a demonstration of field-portable X-ray fluorescence (FPXRF) analyzers. The primary objectives of the demonstration were to (1) determine how well FPXRF analyzers perform in comparison to a standard reference method, (2) identify the effects of sample matrix variations on the performance of FPXRF, (3) determine the logistical and economic resources needed to operate these analyzer, and (4) test and validate and SW-846 draft method for FPXRF analysis. The demonstration found that the analyzer was generally simple to operate. It was designed to operate in the intrusive mode only. The SEFA-P Analyzer is an effective tool for field-based analysis of metals contamination in soil. The analyzer can be expected to identify contaminated areas allowing investigation and remediation decision to be made more efficiently on-site, which may reduce the number of samples that need to be submitted for confirmatory analysis. Ownership and operation of the analyzer may require specific licensing by state nuclear regulatory agencies. There are special radiation safety training requirements and costs associated with this type of license.

Environmental Technology Verification Report: Field Portable X-Ray Fluorescence Analyzer.

Spectrace TN 9000 and TN Pb Field Portable X-ray Fluorescence Analyzers. Superfund Innovative Technology Evaluation

Hess, E.; P. Splichal, PRC Environmental Management, Inc., Lenexa, KS, for the U.S. EPA, Las Vegas, NV. National Exposure Research Lab.

Report No: EPA/600/R-97/145; NTIS: PB2001-101802. 124 pp, Mar 1998

In April 1995, the U.S. EPA sponsored a demonstration of field portable X-ray fluorescence (FPXRF) analyzers. The primary objectives of this demonstration were to evaluate the analyzers for (1) their analytical performance relative to standard analytical methods, (2) the influence of sample matrix variations (texture, moisture, heterogeneity, and chemical composition) on performance, (3) the logistical and economic resources needed to operate these technologies in the field, and (4) testing and validation of an SW-846 draft method for FPXRF analysis. Evaluating the FPXRF analyzers for their

reliability, ruggedness, cost, range of usefulness, data quality, and ease of operation was a secondary objective. Both analyzers exhibited precision similar to the reference methods at 5 to 10 times the precision-based method detection limit (MDL) concentration level. As expected, the chromium data generally showed the poorest precision of the primary analytes. Of the four sample preparation steps evaluated, the initial sample homogenization had the greatest impact on data comparability. Site and soil texture did not appear to affect data comparability. Based on the performance of both TN Spectrace analyzers, this demonstration found them to be effective for characterizing the concentration of metals in soil samples. As with all FPXRF analyzers, unless a user has regulatory approval, confirmatory sampling and data correction is recommended when using these analyzers for site characterization and remediation monitoring.

#### Evaluation of Fourier-Transform Microwave Spectroscopy as a Tool for Quantitative Analysis: Signal Stability Considerations

DaBell, Ryan S. (NIST); Pamela M. Chu; Gerald T. Fraser; Richard D. Suenram.

Instrumentation for Air Pollution and Global Atmospheric Monitoring. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4574, p 216-224, 2002

The high spectral resolution of Fourier-transform microwave (FTMW) spectroscopy provides a quick and unambiguous method for identifying multiple analytes in the gas phase. A small-scale FTMW spectrometer has been constructed for use in quantitative analysis. This paper summarizes efforts to identify and categorize sources of signal instability in the FTMW spectrometer.

#### Explosive Ordnance Detection in Land and Water Environments with Solid Phase Extraction/Ion Mobility Spectrometry

Chambers, William B. (Sandia National Labs.); J.M. Phelan; P.J. Rodacy; S. Reber; R.L. Woodfin.

Detection and Remediation Technologies for Mines and Minelike Targets IV. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3710, p 290-298, 1999

Solid phase micro-extraction methods have been combined with Ion Mobility Spectroscopy to provide rapid, sub-parts-per-billion analysis of nitroaromatic compounds such as trinitrotoluene (TNT) and dinitrotoluene (DNT). This paper will describe the field-portable gas sampling systems that are being developed as a means of classifying buried or submerged objects as explosive ordnance.

#### Fiber Optic Affinity Ligand Sensor for Quantification of Petroleum and Bioremediation

Wavering, Thomas A. (Luna Innovations, Inc., Blacksburg, VA); Jennifer L. Elster; Shufang Luo; Mishell K. Evans; Charles Pennington; Roger Van Tassell; Mark E. Jones.

Advanced Environmental and Chemical Sensing Technology. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4205, p 163-169, 2001

This paper presents a novel system incorporating optical fiber long-period grating (LPG)-based sensors for rapid detection of biological targets as a highly responsive, inexpensive instrument for monitoring key environmental parameters for in situ subsurface bioremediation. The sensor allows for highly sensitive, real-time, refractive index measurements. By applying affinity coatings to the fiber surface, specific binding of molecules can be accomplished using swellable polymers or ligand-based affinity coatings. The sensors are highly responsive, low profile, and can be serially multiplexed within a single-ended probe-like arrangement. The developers propose to use the product for site characterization or as a distributed sensor to map contaminant levels at multiple depths over a large area.

Field Evaluation of a Multiple Beam Sampling Strategy for OP-FTIR Spectrometer Monitoring  
Pang, Keone, Thesis, Master of Science, Industrial Hygiene.  
Dept. of Environmental Health, University of Washington, Seattle. 2000

Open-path FTIR spectroscopy is an optical remote sensing technology utilizing infrared light that can be used to identify and quantify air contaminants over long path lengths; however, the device gives measurements in concentration per unit distance (ppm/meters), making it difficult to determine the location of peak contaminant levels. Working under the hypothesis that the location of the peak could be determined by using a multiple beam sampling strategy, a unistatic OP-FTIR beam path was broken into five segments with multiple mirrors to determine the location of peak styrene concentrations in a boat manufacturing plant. A single gaussian reconstruction of the FTIR measurements was compared against styrene concentrations that were measured by charcoal passive badges and sorbent tubes. A double gaussian reconstruction of the FTIR measurements was explored also. The single gaussian reconstructions of the FTIR measurements tended to follow the ray traces of the passive badge and sorbent tube data. However, the magnitude of the FTIR reconstructed styrene peaks were four to five times larger than the levels determined by the point samplers. In future studies, FTIR measurements should be compared with direct reading instruments, and the distance between the FTIR beam path and point-sampling units should be kept to a minimum.

Field-Portable, Fast GC/TOFMS

Syage, Jack (Syagen Technology, Inc.); Brian Nies; Rick Harkewicz.  
The 3rd Harsh-Environment Mass Spectrometry Workshop, 25-28 March 2002 Pasadena, California.

A man-portable, fast gas chromatograph, time-of-flight mass spectrometer (GC/TOFMS) is designed to meet performance, size, weight, power, cost, and ruggedness requirements for a laboratory in the field. The core technology can be adapted to specific applications, e.g., real-time point detection for hazardous chemical releases or chemical weapons, biological agent signature identification, and mobile monitoring platforms. Progress has been made in integrating a low-power, high-speed GC with the capability for accurately recording fast GC transients for targeted compound detection using a photoionization (PI) source coupled to a quadrupole ion trap, time-of-flight (QitTof) instrument. The system specifications are 40 lb weight, 2 cu feet in size, and 150 W of power consumption. The instrument records mass spectra at nominally 60 Hz (USA) making it suitable for fast GC. The GC is temperature programmable and can cycle typical samples in 120 to 240 s. Preliminary GC measurements gave baseline resolution with peak widths of about 1 s and detection limits of about 20-100 ppb and 10-50 pg. We also present results on a pyrolysis/GC front end showing distinct signature peaks for biological bacteria and spore detection. This work is being supported by the U.S. Army for chemical and biological defense.

<http://cot.marine.usf.edu/hems/workshop/3rdworkshop/program.htm>

Field-Portable Laser-Diode Spectrometer for the Ultra-Sensitive Detection of Hydrocarbon Gases  
Gibson, Graham M. (Univ. of Glasgow); Stephen Monk; Miles J. Padgett.

Optical Spectroscopic Techniques, Remote Sensing, and Instrumentation for Atmospheric and Space Research IV. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4485, p 244-249, 2002

The researchers have developed a field-portable optical gas sensor for the ultra-sensitive detection of ethane. The system is based on an adaptation of a commercially available system with a cryogenically cooled, lead-salt, laser diode at 3.34 microns and a multi-pass astigmatic Herriott sample cell. The system has been adapted to a second derivative wavelength modulation scheme giving a lower detection



limit of less than 100 parts per trillion in a one-second measurement time. Every aspect of the instrument's operation is controlled by custom-designed software.

#### First Field Test of NAPL Detection with High Resolution Borehole Seismic Imaging

Geller, J.T. (LBNL); J.E. Peterson; K.H. Williams; J.B. Ajo-Franklin; E.L. Majer.

9th Biennial International Conference on Nuclear and Hazardous Waste Management, 4-8 August 2002, Reno, NV. Paper No: LBNL-50689, 6 pp, May 2002

A field test was conducted to evaluate the detectability of NAPLs by high resolution tomographic borehole seismic imaging at a former DOE manufacturing facility in Pinellas County, FL. Cross-hole seismic and radar measurements were made in a shallow aquifer contaminated with non-aqueous phase liquids (NAPLs). Cone penetration test (CPT) and induction logging were performed for lithology and conductivity, respectively. The main challenge is to distinguish fluid phase heterogeneities from anomalies arising from geologic structure. The approach compared measurements between locations of known contamination with a nearby uncontaminated location of similar lithology where differences in signal transmission were attributed to fluid phase changes. The CPT data show similar lithologic structure at the locations both within and outside the NAPL-contaminated area. Zones of low seismic amplitude at about 7 m depth appeared more extensive in the NAPL-contaminated area. These zones may be the result of fluid phase heterogeneities (NAPL or gas), or they may be due to the lithology, i.e. attenuating nature of the layer itself, or the transition between two distinct layers. The presence of lithologic contrasts, specifically from higher permeability sands to lower permeability silts and clays, also indicate potential locations of NAPL, as they could be flow barriers to downward NAPL migration.

[http://www.osti.gov/bridge/product.biblio.jsp?osti\\_id=797864](http://www.osti.gov/bridge/product.biblio.jsp?osti_id=797864)

#### Fourier Transform Spectrometry

Davis, Sumner P.; Mark C. Abrams; James W. Brault.

Academic Press, Orlando, FL. ISBN: 0120425106. 2001

This presentation enables readers to obtain a clear understanding of Fourier transform spectrometry (FTS), which can be crucial to research. Due to the increasing complexity and commercialization of instrumentation, achieving optimum performance in research applications and automated usage can be challenging. For example, a thorough understanding of the instrument can dramatically affect the outcome of the experiment and the generation of reliable data in applications where conditions are not ideal and resulting signals are weak. This book provides a comprehensive discussion of FTS from the ground up, covering basic concepts, instrumentation, data-processing algorithms, and techniques for computerized spectral analysis.

#### Fuels in Soil Test Kit: Field Use of Diesel Dog® Soil Test Kits. Topical and Final Report

Sorini, Susan S.; John F. Schabron; Joseph F. Rovani, Jr., Western Research Inst., Laramie, WY.

Report No: WRI-02-R018, 41 pp, Sep 2002

Western Research Institute (WRI) has developed a new commercial product ready for technology transfer, the Diesel Dog® Portable Soil Test Kit, for performing analysis of fuel-contaminated soils in the field. The technology consists of a method developed by WRI (U.S. Patents 5,561,065 and 5,976,883) and hardware developed by WRI that allows the method to be performed in the field (patent pending). The method is very simple and does not require the use of highly toxic reagents. The aromatic components in a soil extract are measured by absorption at 254 nm with a field-portable photometer. WRI added significant value to the technology by taking the method through the American Society for

Testing and Materials (ASTM) approval and validation processes, which resulted in ASTM Method D 5831-96, Standard Test Method for Screening Fuels in Soils. This ASTM designation allows the method to be used for federal compliance activities. In June 2001, the Diesel Dog technology won an American Chemical Society Regional Industrial Innovations Award. To gain field experience with the new technology, Diesel Dog kits have been used for a variety of site evaluation and cleanup activities. Information gained from these activities has led to improvements in hardware configurations and additional insight into correlating Diesel Dog results with results from laboratory methods. The Wyoming Department of Environmental Quality (DEQ) used Diesel Dog Soil Test Kits to guide cleanups at a variety of sites throughout the state. ENSR of Acton, MA, used a Diesel Dog Portable Soil Test Kit to evaluate sites in the Virgin Islands and Georgia. ChemTrack and the U.S. Army Corps of Engineers successfully used a test kit to guide excavation at an abandoned FAA fuel-contaminated site near Fairbanks, AK. Barenco, Inc., is using a Diesel Dog Portable Soil Test Kit for site evaluations in Canada, and the kit was used at the cleanup of a small spill of diesel fuel in Laramie, WY.  
[http://www.osti.gov/bridge/product.biblio.jsp?osti\\_id=803199](http://www.osti.gov/bridge/product.biblio.jsp?osti_id=803199)

Gas Monitoring in the Process Industry Using Diode Laser Spectroscopy  
Linnerud, Icar; Peter Kaspersen; Tycho Jæger, Norsk Elektro Optikk A/S, Skarer, Norway.  
Applied Physics B: Lasers and Optics, Vol 67, p 297-305, 1998

Tunable diode laser absorption spectroscopy in the near infrared can be used to monitor gases reliably and with little maintenance required. This paper presents a brief description of monitors that use high frequency wavelength modulation spectroscopy with second harmonic detection, with a discussion of typical applications and the problems related to them, e.g., line broadening effects and frequency drift of diode lasers.  
[http://www.neo.no/applied\\_phys.html](http://www.neo.no/applied_phys.html)

Ground-Based Passive FT-IR Spectrometry  
Knapp, Robert B.; R.J. Combs; R.T. Kroutil, U.S. Army Edgewood Chemical Biological Ctr.  
Vibrational Spectroscopy-based Sensor Systems. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4577, p 269-286, 2002

A ground-based passive FT-IR spectrometry system acquired absorbance and transmittance spectra for industrial stack evaluations and open-air controlled vapor-generation experiments. Sulfur dioxide and nitrous oxide were detected from a coal-burning power plant and an acid plant, respectively, with both MWIR and LWIR passive sensors. The controlled open-air experiments relied on only a LWIR sensor. This paper describes the monitoring results.

Guide for Characterization of Sites Contaminated with Energetic Materials  
Thiboutot, Sonia (Defence Research Establishment Valcartier (DREV), Val-Belair, Quebec, Canada),  
Guy Ampleman; Alan D. Hewitt (U.S. Army Cold Regions Research and Engineering Laboratory (CRREL), Hanover, NH).  
Report No: ERDC/CRREL TR-02-1, 58 pp, Feb 2002

Production and firing of munitions, demolition procedures, and destruction of outdated ammunition can all cause dispersion of energetic compounds into the environment. These various scenarios lead to different patterns of contamination, thereby creating a need for a general protocol that is applicable in all circumstances. The goal of this guidance document is to collate information relevant to the characterization of sites contaminated by energetic materials and serve as a reference for future sampling campaigns on sites potentially contaminated with explosives. The characterization of training

and firing ranges, demolition, and open burning/open detonation ranges will allow assessment of the environmental impacts of these various operational activities. In addition, it will provide information critical to the establishment of future operational requirements and procedures that minimize environmental damage.

<http://www.crrel.usace.army.mil/library/pub02fyo.htm>

#### A High-Performance Handheld Gas Chromatograph

Yu, Conrad M., Lawrence Livermore National Laboratory.

The 3rd Harsh-Environment Mass Spectrometry Workshop, 25-28 March 2002 Pasadena, California.

One of the hot topics in the analytical instrumentation community is the need to move analysis away from the laboratory to the field, where the samples are, to enable quicker real-time data collection and lower analysis cost. A recent improvement on a hand-held gas chromatograph involves a sample pre-concentrator unit and related electronics to improve the detection capability of trace chemical components in air. The prototype unit originally was developed at the Micro-Technology Center of Lawrence Livermore National Laboratory by means of Micro-Electro-Mechanical-System (MEMS) technology. The total weight of this 8" x 5" x 3" hand-held gas chromatograph is about 8 lbs. It consumes about 12 watts of electrical power and produces a response in about two minutes. The new detector is a Glow Discharge detector with a sensitivity of parts per billion and an average retention time of about 30 to 45 seconds. Under optimum condition, the calculated effective plate number for the MEMS silicon column is about 40K. The separation column in the portable GC is fabricated completely on silicon wafers. Silicon is a good thermal conductor and it provides a uniform temperature for the whole column together with the possibility of rapid heating and cooling of the column. The operational temperature can be as high as 350 degrees Celsius (maximum column coating temperature). The GC system is capable of rapid column temperature ramping and cooling operations. These capabilities are especially important for organic and biological analyses in GC applications.

<http://cot.marine.usf.edu/hems/workshop/3rdworkshop/program.htm>

#### A Highly Selective Fluorescent Chemosensor for Lead Ions

Chen, Chao-Tsen; Wan-Pei Huang.

Journal of the American Chemical Society, Vol 124 No 22, p 6246 6247, Jun 2002

A chemosensor has been prepared by the condensation of 4-(N,N-diethylamino)salicylaldehyde with the  $\beta$ -ketoester appended with 15-monoazacrown-5 ether in the presence of piperidine. Absorption and fluorescence emission titrations of the sensor with alkali, alkaline-earth, and heavy-metal ions performed in acetonitrile at room temperature indicate that there are no changes in the presence of monovalent ions, but red-shift absorptions are observed in the absorption or fluorescence emission spectra of the divalent ions. The titration results of the sensor indicate a 40-fold fluorescence enhancement for lead, for which the sensor exhibits a particularly high affinity and selectivity.

#### The Improved Teeny-TOF Mass Spectrometer for Chemical and Biological Sensing

Ecelberger, Scott A. (Johns Hopkins Univ. Applied Physics Lab); T.J. Cornish; W.A. Bryden.

The 3rd Harsh-Environment Mass Spectrometry Workshop, 25-28 March 2002 Pasadena, California.

A miniature, low voltage, reflectron time-of-flight mass spectrometer has been developed and tested on a series of compounds ranging in mass from a few hundred Da to over 50kDa. The design employs a small and commercially available 10 l/s pump, a 140uJ nitrogen laser, and fiber optics to deliver the laser energy. A gridless, focusing ion source is operating at 4.5kV, the ruggedized reflector is rolled from a flexible circuit board and encased in fiberglass, and the detector has an improved anode that

reduces ringing commonly found in coaxial designs. The first prototype is currently being tested for its use in chemical and biological threat detection.

<http://cot.marine.usf.edu/hems/workshop/3rdworkshop/program.htm>

#### In Situ Multiplexing Long-Path Fiber Optic Remote Sensing System of Methane with Single Laser Source

Yin, Wang-bao (Shanxi Univ.); J.-M. Zhao; C.-Y. Li; L. Xiao; S. Jia.

Advanced Sensor Systems and Applications. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4920, p 240-246, 2002

A laboratory prototype of a cost-effective, multiplexing, fiber-optic remote monitoring system has been demonstrated for the measurement of the spatial distribution of methane and other gases in a wide area. The remote detection system is based on frequency-modulation spectroscopy and harmonic detection. By means of a fiber-optic splitter, the sensor employs a single laser source to get multicenter measurement in the near IR region. The new system performs with increased reliability and sensitivity when compared with a commercially available system. The researchers foresee its use in areas such as landfill sites, mines, and urban and residential areas.

#### Imaging and Characterisation of Subsurface Solute Transport Using Electrical Resistivity Tomography (ERT) and Equivalent Transport Models

Kemna, A.; J. Vanderborght; B. Kulessa; H. Vereecken.

Journal of Hydrology, Vol 267 No 3-4, p 125-146, Oct 2002

A field tracer experiment was conducted at the Krauthausen test site in Germany. The spatial and temporal evolution of an injected NaBr solute plume was monitored in a 2-dimensional electrical resistivity tomography (ERT) image plane for 90 days. ERT maps changes in bulk electrical conductivity.

#### Immunoaffinity-Based Phosphorescent Sensor Platform for the Detection of Bacterial Spores

Scholl, Peter F. (Johns Hopkins Univ.), C.B. Barger, T.E. Phillips; T. Wong (Army Research Lab.); S. Abubaker (Johns Hopkins Univ.), J.D. Groopman, P.T. Strickland, R.C. Benson.

In-Vitro Diagnostic Instrumentation. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3913, p 204-214, 2000

This paper proposes an inexpensive, simple, and rapid means of spore detection by non-specialists in emergency situations, such as an attack with biological weapons (e.g., anthrax). The feasibility of the concept was demonstrated by the immunoaffinity capture of spores of the anthrax simulant *B. globigii* on a column, followed by their washing, elution, and phosphorescent detection. The method rapidly detects spores generically via the rapid extraction of dipicolinic acid (DPA) followed by its chelation with terbium to yield a phosphorescent complex. The researchers evaluated the speed and efficacy of chemical, thermal, and mechanical methods of DPA extraction. It is estimated that implementation of the study results will permit development of a device requiring 3-5 minutes per analysis with a limit of detection on the order of 500 ng spore/mL.

#### Infrared Cavity Ringdown and Integrated Cavity Output Spectroscopy for Trace Species Monitoring

Paul, Joshua B. (Los Gatos Research), J.J. Scherer, A. O'Keefe; L. Lapson (Harvard Univ.), J.R.

Anderson; C.F. Gmachl (Lucent Technologies/Bell Labs), F. Capasso, A.Y. Cho.

Vibrational Spectroscopy-based Sensor Systems. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4577, p 1-11, 2002

The researchers report how off-axis optical paths through high finesse optical cavities can be employed to produce relatively simple spectrometers capable of ultrasensitive absorption measurements. A proof-of-concept study using visible diode lasers has achieved a normalized absorption sensitivity of  $1.8 \times 10^{-10} \text{ cm}^{-1} \text{ Hz}^{-1/2}$ , and quantum cascade lasers have been employed to extend this method into the mid-infrared region, to sensitivities of  $1.2 \times 10^{-9} \text{ cm}^{-1} \text{ Hz}^{-1/2}$ .

Infrared Hyperspectral Tunable Filter Imaging Spectrometer for Remote Leak Detection, Chemical Speciation, and Stack/Vent Analysis Applications

Hinnrichs, Michele, Pacific Advanced Technology.

Instrumentation for Air Pollution and Global Atmospheric Monitoring. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4574, p 144-152, 2002

Based on the advances in hyperspectral tunable filter technology, Pacific Advanced Technology is developing a small field-portable infrared imaging spectrometer (nicknamed Sherlock) for detection of fugitive gas leaks. The system uses Pacific Advanced Technology's Image Multi-spectral Sensing (IMSS) diffractive optic tunable filter. Sherlock has an embedded digital signal processor for real-time detection of the gas leak while surrounded by severe background noise. The infrared sensor engine is a  $256 \times 320$  midwave cooled focal plane array that spans the spectral range from 3 to 5 microns, ideal for most hydrocarbon leaks. This paper describes the design of the prototype Sherlock camera and discusses the data collected from measurements at a gas processing plant and a kiln. This work is supported by U.S. DOE, the State of California, and the Gas Technology Institute.

Innovative Remote Sensing Applications for Environmental Management of a Military Training Area  
Klemm, Horst G. (IAB GmbH); Albert Boehm (U.S. Army CMTC/Hohenfels); Karl Segl (GeoForschungsZentrum Potsdam).

Remote Sensing for Environmental Monitoring, GIS Applications, and Geology. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4545, p 24-34, 2002

This paper presents a recent project in which hyperspectral reflectance data were used to determine mineral content in soils and differentiate surface cover types using a new unmixing approach. The innovative remote sensing project showed the high potential of hyperspectral imagery for examination of soils and surface cover types, which will be useful to DoD's need for information to support environmental management.

Innovative Techniques to Investigate Contamination in Fractured Bedrock

Gaule, C. (Malcolm-Pirnie, Inc., Albany, NY); K. Goldstein (Malcom-Pirnie, White Plains, NY); G. Anderson (U.S. Army Corps of Engineers, Baltimore, MD).

2001 International Containment & Remediation Technology Conference & Exhibition, 10-13 June 2001, Orlando, Florida. Conference Program. University of Florida, Tallahassee. Abstract 155, p 78, 2001

Watervliet Arsenal in Watervliet, NY, is the United States' oldest continuously operating cannon manufacturing facility. The extent of ground-water contamination at the Arsenal was investigated through the installation of traditional ground-water monitoring wells along with innovative investigative techniques. During the first two phases of the investigation, ground-water monitoring wells were installed at the watertable and the intermediate bedrock. The highest concentrations of metals and dense

non-aqueous phase liquids (DNAPLs) were detected at the discharge boundary at approximately 110 feet below the ground surface. The later phases of well installation were focused through the use of borehole geophysical techniques such as temperature and resistivity logging, traditional video logging, and the relatively new technique of an enhanced digital borehole imaging processing system (BIPs). The BIPs allowed the determination of fracture orientation, fracture aperture width, and frequency, which helped target placement of the third phase of wells. The results of the third phase of the investigation indicated that the contaminants extended more than 160 feet below the ground surface. Additional borehole geophysical logging techniques helped further define the high flow zones in the contaminated bedrock. These techniques included acoustic televiewer, electro-magnetic (EM), and heat pulse flowmeter under pumping conditions. Heat pulse flowmeter is very accurate and can define the active fractures within the system to 0.01 gallons per minute. The methods were combined in the field in a cross-borehole configuration to determine the degree of interconnection between wells. The combined methods replaced conventional long-term pumping tests. The data collected through these methods were used for the calculation of mass flux to the Hudson River.

Integrated Geophysical and Hydraulic Investigation to Characterize a Fractured-Rock Aquifer, Norwalk, Connecticut

Lane, J.W. (U.S. Geological Survey, Hartford, CT); J.H. Williams; C.D. Johnson; D.M. Savino; F.P. Haeni.

Report No: USGS/WRI-001-4133; NTIS: PB2002-106823, CD-ROM [97 pp], 2002

This report presents results of an integrated geophysical and hydraulic investigation to characterize a contaminated fractured-bedrock aquifer site in Norwalk, Connecticut. The USGS conducted the investigation as part of a Cooperative Research and Development Agreement with United Technologies Corporation to develop and test geophysical methods to investigate bedrock hydrogeology and to monitor active and innovative remediation measures. The purpose of this geophysical and hydraulic investigation was to characterize the bedrock lithology and structure at the site and to identify the orientation, distribution, and hydraulic characteristics of fractures and transmissive zones in the fractured-bedrock aquifer. This work supported ongoing efforts to develop a conceptual site model of ground-water flow and solute transport and to design a discrete-zone monitoring (DZM) and sampling network.

An Integrated, Stacked Microlaboratory for Biological Agent Detection with DNA and Immunoassays  
Yang, J.M.; J. Bell; Y. Huang; M. Tirado; D. Thomas; A.H. Forster; R.W. Haigis; P.D. Swanson; R.B. Wallace; B. Martinson; M. Krihak, Nanogen, Inc., San Diego, CA.

Biosensors and Bioelectronics, Vol 17 No 6-7, p 605-618, Jun 2002

Researchers have developed an integrated, stacked microlaboratory for performing automated electric-field-driven immunoassays and DNA hybridization assays. The stacked microlaboratory was fabricated by ordered lamination of several different functional layers (all 76 x 76 mm<sup>2</sup>) including a patterned polyimide layer with a flip-chip bonded CMOS chip, a pressure sensitive acrylic adhesive (PSA) layer with a fluidic cutout, an optically transparent polymethyl methacrylate (PMMA) film, a PSA layer, a patterned polyimide layer with a flip-chip bonded silicon chip, a PSA layer with a fluidic cutout, and a glass cover plate layer. Potential applications of the integrated microlaboratory include genetic identification and detection of bacteria and biological warfare agents.

Integrated Surface Acoustic-Wave and Semiconducting-Metal-Oxide Sensor Array

Smith, Dean J. (Sensor Research and Development Corp.); J.M. Hammond; T. Mlsna; M. Hutchinson; C. Brown; B. Oickle.

Internal Standardization and Calibration Architectures for Chemical Sensors. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3856, p 97-108, 1999

A novel sensor approach incorporates two sensing techniques, surface acoustic wave (SAW), and semiconducting metal oxide (SMO), into an array of arrays. This integrated sensor array can provide marked improvements over either array alone in the increased bandwidth of measurands, the capability of cross-verifying results with complementary sensor technology responses, and performance in the presence of interferences. This paper focuses on aspects of sensor selection, sensor data collection, manipulation, management, and processing for an integrated SAW and SMO sensor array.

Introduction to Environmental Analysis

Reeve, Roger.

John Wiley & Sons, Inc., New York. ISBN: 0-471-49294-9. 323 pp, 2002

This publication provides information on the application of analytical techniques such as gas chromatography (GC), liquid chromatography (LC), infrared (IR), and x-ray fluorescence (XRF) for analyzing and measuring water, solid, and atmospheric samples and for monitoring environmental pollutants. The text also includes sections on solid and liquid extraction techniques. Field analysis is emphasized, reflecting the growing application of rapid turnaround techniques. The information on sampling strategies reflects considerable growth in this area. An online version of this title is available for license through Wiley InterScience.

Investigation Methods For Contaminated Fractured Aquifer

Bardenhagen, Ingo; Jorg Goedicke, Peschla + Rochmes GmbH, Hertelsbrunnenring, Kaiserslautern, Germany.

Investigacion, Gestion y Recuperacion de Acuiferos Contaminados, Oct 2001, Alicante, Spain.

Inst. of Geology and Mineralogy of Spain, Ministry of Science and Technology, Madrid, Spain.

p 105-116, 2001

Investigations of contaminated aquifers often are concentrated too much on the plume, when the need for fundamental knowledge of the fractured aquifer itself calls for a more detailed investigation. This paper discusses investigation tools that were combined in the determination of a fracture system in the Buntsandstein aquifer in south-western Germany. The aquifer is contaminated by fuel and chlorinated hydrocarbons. Core drilling and geophysical logging, including sonic logs, fluid logging, packer tests, and pumping tests, allowed investigators to develop a detailed model of the aquifer before implementing a remediation scheme. [This is one of 11 papers in English out of 36 papers delivered at a Spanish-language conference.]

[http://www.igme.es/internet/web\\_aguas/igme/publica/lib15.htm](http://www.igme.es/internet/web_aguas/igme/publica/lib15.htm)

Ion Trap Secondary Ion Mass Spectrometry: Moving Toward Fieldable Systems

Appelhans, Anthony D.; J.E. Olson, Idaho National Engineering and Environmental Lab.

The 3rd Harsh-Environment Mass Spectrometry Workshop, 25-28 March 2002 Pasadena, California.

Adsorption of chemical contaminants on solid surfaces presents a difficult challenge for both detection and decontamination because many chemical weapons can bind tightly to a surface, resisting extraction or degradation, and can change form into equally toxic compounds while on the surface, confounding detection technologies tuned only to the agent compound. Means are sought to determine, once the volatile components have dispersed, how to tell if the agent or its toxic byproducts remain on the surface, steps, handrails, or benches. Ion trap secondary ion mass spectrometry (ITSIMS) has been

applied for detecting and characterizing trace levels of a variety of complex compounds on surfaces. In most cases the goal is simple detection and chemical identification. Past experience has demonstrated that levels down to 0.001 monolayer can be detected on many type of environmental samples, such as soil, leaves, minerals, and concrete . In previous studies involving the detection of the nerve agent VX on different substrates, it was noted that the degradation of the VX was highly dependent upon the substrate. For sandy soils, degradation was extremely slow (months), while for concrete samples the degradation was rapid (hours). For obvious reasons the lifetime of such compounds on different surfaces is an important factor in making operational decisions in the field, and thus there is impetus to develop field-transportable systems. This paper summarizes progress in the development of field-transportable ion trap SIMS.

<http://cot.marine.usf.edu/hems/workshop/3rdworkshop/program.htm>

Issues Involved in Using Sol-Gel-Derived Glasses as Platforms for Chemical Sensing

Doody, Meagan A. (SUNY/Buffalo); G.A. Baker; S. Pandey; N.J. Bonzagni; F.V. Bright.

Internal Standardization and Calibration Architectures for Chemical Sensors. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3856, p 2-10, 1999

This paper outlines the challenges the researchers have faced in exploring the potential of sol-gel-derived glasses as platforms for advanced sensors and biosensors, with particular attention to the performance of polyclonal anti-dansyl antibodies sequestered within a series of xerogels. The study assessed antibody performance by determining the hapten/antibody association constant, the static excitation and emission for the dansyl hapten bound to the antibody combining site, and the excited-state fluorescence anisotropy and intensity decay kinetics for the dansyl/anti-dansyl system within a series of xerogels.

Long-Path Optical Spectral AOTF-Based Gas Analyzer

Pozhar, Vitold E.; V.I. Pustovoit, Scientific Technological Ctr. of Unique Instrumentation.

Instrumentation for Air Pollution and Global Atmospheric Monitoring. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4574, p 174-178, 2002

The authors describe a long-path spectral acousto-optical tunable filter (AOTF)-based gas analyzer and compare the results of performance tests with those obtained from tests with other differential optical absorption spectroscopy (DOAS) gas analyzers. The advantages of using AOTF as a spectral selective element are discussed.

Mapping and Monitoring Complex Chemical Components in Ambient Air using Fast GC/MS and Multivariate Data Analysis

Meuzelaar, Henk; Neil S. Arnold, Univ. of Utah.

The 3rd Harsh-Environment Mass Spectrometry Workshop, 25-28 March 2002 Pasadena, California.

It is well recognized that the inherently poor transmission of optical, microwave and radio signals in U/W environments severely limits the use of the kind of stand-off spectroscopic techniques for rapid area mapping that have been so spectacularly successful in astronomy and space science. Consequently, the new generation of fast, miniaturized, multidimensional point detectors (including a wide range of MS-based techniques), promises to provide a powerful alternative, whether deployed as fixed-grid distributed sensor systems or on fast roving (robotic and/or remotely controlled) platforms.

<http://cot.marine.usf.edu/hems/workshop/3rdworkshop/program.htm>



Mapping Minerals at the Copper Flat Porphyry, New Mexico, Using AVIRIS Data  
Verdel, C.S.; D. Knepper, Jr.; K.E. Livo; V.T. McLemore; B. Penn; R. Keller.  
AVIRIS Airborne Geoscience Workshop Proceedings 2001. Jet Propulsion Laboratory, California Inst.  
of Technology. 7 pp, 2001

The Copper Flat porphyry is a Laramide copper deposit in southwest New Mexico. High-altitude AVIRIS data were acquired over the site in 1998. Limonite minerals, carbonates, some phyllosilicates, epidote, gypsum, and tremolite/talc have been preliminarily mapped based on AVIRIS data. The results indicate a fairly regular zonation of hydrothermal alteration minerals around the porphyry that is consistent with classic models of alteration from porphyry copper deposits. Verification of the preliminary results is on-going. X-ray diffraction analyses and laboratory spectral analyses will be performed on samples from the area to confirm the results of mineral mapping.  
[http://popo.jpl.nasa.gov/docs/workshops/01\\_docs/toc.html](http://popo.jpl.nasa.gov/docs/workshops/01_docs/toc.html)

Measurement of Ethanol Concentration with Near IR Diode Lasers  
Berezin, A. (General Physics Inst., Moscow, Russia); Y. Bugoslavskii; O. Ershov; V. Kutnyak; A. Nadezhdinskii.  
TDLS 98: 2nd International Conference on Tunable Diode Laser Spectroscopy, 6-10 July 1998,  
Moscow, Russia. Book of Abstracts, p 34, 1998

In an attempt at distant detection of alcohol vapor in the open atmosphere with a diode laser (DL) spectroscopy technique, the DL was driven by current pulses of sawtooth form, and a small portion of the gas absorption spectrum was compared with a reference spectrum. The gas concentration was calculated as correlation function between reference and detected portions of spectra. The diode laser developed for ethanol measurements included two cells filled with ethanol-air gas mixtures at different concentrations and pressures. One of the cells was just a tube cell 2 meters in length; the second cell was a tuneable White multipass cell with optical path length from 0.8 to 30 meters. The detection limit of the spectrometer for ethanol on a 3-meter optical path was found to be 50 ppm in open atmosphere.

MEMS-Based Sensor System for Environmental Monitoring  
Daly, J.T. (Ion Optics, Inc.), E.A. Johnson, N. Moelders, M.P. McNeal, M.U. Pralle, A.C. Greenwald, W. Ho, I. Puscasu; T. George (Jet Propulsion Lab.), D.S. Choi.  
Advanced Environmental Sensing Technology II. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4576, p 49-55, 2002

The authors introduce a new IR-based sensor technology for environmental monitoring of industrial pollutants, such as CO<sub>2</sub>, CO, and NO<sub>x</sub>. The design concept exploits Si-based, thermally isolated suspended bridge structures that function as both IR emitter and detector. Photonic bandgap (PBG) modified surfaces enable narrow band IR emission for high chemical selectivity and sensitivity. Spectral tuning is done by controlling symmetry and lattice spacing of the PBG structures. Non-dispersive infrared (NDIR) spectroscopic techniques were used for gas detection, and target gas species and concentrations were determined from comparison to reference spectra. The sensor system has been demonstrated on CO<sub>2</sub> gas, and a multi-channel microsensor-array is proposed for multigas detection.

MEMS Optical Assemblies and Microscopes  
Descour, Michael (Optical Sciences Center, Univ. of Arizona), J.D. Rogers, J. Lee; Ari H.O. Karkkainen (VTT, Oulu, Finland).  
In Situ Instruments Workshop, 11-13 June 2002, Pasadena, California. NASA, Jet Propulsion Laboratory, Center for In-Situ Exploration and Sample Return.

The authors discuss prospects for miniaturized imaging and sensing devices such as a microscope on a chip and a spectrometer on a chip. The paper reviews ongoing work and discusses future concepts for micro-instruments, with particular attention to the prospective fabrication and assembly methods that will enable such devices.

#### Metal Mine Rock and Waste Characterization Tools: an Overview

Lapakko, Kim, ADTI-MMS, Minnesota Dept. of Natural Resources, St. Paul, MN.

International Inst. for Environment and Development. Publication No 67, 30 pp, Apr 2002

[Posted on the Acid Drainage Technology Initiative - Metal Mining Sector web page at

[www.mackay.unr.edu/adti](http://www.mackay.unr.edu/adti)]

This paper identifies categories of tools available for characterizing mine wastes and predicting drainage quality and enumerates some of the specific tools within these categories, though it is not intended to be a complete catalog of tools nor to describe those included in great detail. The analytical focus of the tools ranges from screening large areas of abandoned mine wastes to determining compositions of individual mineral grains. A brief summary of mine waste drainage chemistry is provided as background to the subsequent discussion.

[http://www.iied.org/mmsd/mmsd\\_pdfs/067\\_mftf-f\\_lapakko.pdf](http://www.iied.org/mmsd/mmsd_pdfs/067_mftf-f_lapakko.pdf)

or

<http://www.mackay.unr.edu/adti/workbook5.pdf>

#### Methods Manual for Detection of Propellant, Explosive, or Pyrotechnic Compounds

U.S. Army Environmental Center.

This web page lists the contents of the Manual and provides the text of the following methods in html format: EPA Method 4050 (Screening Procedure to Determine TNT Explosives in Water and Soil by Immunoassay); EPA Method 4051 (Screening Procedure to Determine RDX in Soil and Water by Immunoassay); EPA Method 7580 (Determination of White Phosphorus (P4) Concentration by Solvent Extraction and Gas Chromatography); EPA Method 8330 (Determination of Concentration of Nitroaromatics and Nitramines by High-Performance Liquid Chromatography (HPLC)); and EPA Method 8510 (Field Method for Screening for Concentrations of RDX in Soil).

<http://www.crrel.usace.army.mil/techtransfer/products/pepmanual/>

#### Microfabrication of Cylindrical Ion Trap Mass Spectrometer Arrays

Short, Tim (Center for Ocean Technology, Univ. of South Florida), D. Fries, G.P.G. Kibelka; H.

Peddananikalva, S. Bhansali (Dept. of Electrical Engineering, Univ. of South Florida).

The 3rd Harsh-Environment Mass Spectrometry Workshop, 25-28 March 2002 Pasadena, California.

This paper describes progress in the design, fabrication and testing of cylindrical ion trap (CIT) arrays using two separate microfabrication approaches. One approach involves deep reactive ion etching (DRIE) of silicon to form arrays of "ring electrode" holes and endplate structures. These structures will be metallized to create conducting surfaces and then bonded, with insulating layers between them, to form monolithic CIT array devices. A separate approach uses micro-electric discharge machining (micro-EDM) of metal plates to form the "ring electrode" and endplate structures, and subsequent bonding with insulating layers to form the CIT arrays. A key feature in both designs will be use of microfabricated endplates that provide high transmission rigid grid-structures for each CIT of the array. This construction should optimize electron and ion transmission into and out of the CIT, while providing high-quality electric field definition within each CIT.

<http://cot.marine.usf.edu/hems/workshop/3rdworkshop/program.htm>

### Microfluidics in Environmental Monitoring: Toward a Shoebox-size Spectrometer for Measuring Mercury in the Environment

Vander Wilp, William (Univ. of Waterloo, Waterloo, ON, Canada); Vassili Karanassios.

Advanced Environmental and Chemical Sensing Technology. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4205, p 119-127, 2001

This paper describes steps taken toward the development of a portable shoebox-size spectrometer for measuring mercury in the environment to obtain results on-site in near real time.

### Microphotonic Sensors for the Rapid Detection of the Presence of Explosive Gas Mixtures

McNesby, Kevin L. (Army Research Lab.); Andrzej W. Miziolek.

Vibrational Spectroscopy-Based Sensor Systems. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4577, p 262-268, 2002

Scientists at the U.S. Army Research Laboratory have developed a first-generation, microphotonic sensor for rapid (10 ms response time) measurement of vapors from the hydrocarbon-based fuels JP-8, DF-2, and gasoline. The sensor is based on a laser mixing technique that uses two tunable diode lasers emitting in the near-infrared spectral region to measure concentrations of gases having unstructured absorption spectra. The fiber-mixed laser beam consists of two wavelengths, one that is absorbed by the fuel vapor and one that is not. By sinusoidally modulating the power of the two lasers at the same frequency but 180 degrees out of phase, a sinusoidal signal is generated at the detector in line of sight with the target gas. The signal amplitude is proportional to fuel vapor concentration. A second-generation sensor, designed to measure the full envelope of the first overtone C-H vibrations in middle distillate fuels, is under development.

### Microporous Layer for Selective Detection of VOCs in Gases and Liquids

Belge, Georg (Univ. of Tuebingen, Tuebingen, Germany), Dirk Nopper, Martin Herold, Guenter Gauglitz; R. Buchold (Dresden Univ. of Technology, Dresden, Germany), Gerald Gerlach.

Advanced Environmental and Chemical Sensing Technology. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4205, p 84-92, 2001

A sensitive layer of a microporous polymer with molecular sieving properties is introduced in a sensor array, enhancing the discrimination capabilities of the sensing method tremendously. The size-selective sensitive layers of the glassy polymer can discriminate analytes that are bigger or smaller than the mean pore size. By controlling an analyte's mobility into sensing matrix, microporous polymers make it possible to extend the sensitivity spectrum for chemical sensors.

### Miniature Local Electrode Atom Probe

Robert Kowalczyk, Kimberly R. Kuhlman, Jennifer Ward, Victor White, Beverley Eyre, Pamela G. Conrad (Jet Propulsion Laboratory); Neal D. Evans, Michael K. Miller (Oak Ridge National Laboratory); Richard Martens, Jesse Olson, Thomas F. Kelly (Imago Scientific Instruments).

In Situ Instruments Workshop, 11-13 June 2002, Pasadena, California.

NASA, Jet Propulsion Laboratory, Center for In-Situ Exploration and Sample Return.

The Miniature Local Electrode Atom Probe (Mini-LEAP) will be capable of performing in situ three-dimensional analyses with near atomic spatial resolution and mass spectroscopy with high mass resolution. The LEAP is a new analytical instrument based on the Field Ion Microscope (FIM), which utilizes a rapidly pulsed, highly localized electric field to evaporate a needle-shaped specimen, one atom

at a time. The ions are accelerated into a two-dimensional detector with single ion sensitivity. The mass-to-charge ratio is determined by measuring the time of flight. Pulsing the sample at a rate of 10 kHz at a 5% evaporation rate yields 500 ions per second, or 1.8 million ions per hour. A database stores the x, y, and z positions and mass-to-charge ratio of each atom from which the sample's three-dimensional structure and composition can be reconstructed at the near atomic scale.

#### Miniature TOF Mass Spectrometer Using a Flexible Circuitboard Reflectron

Cornish, Tim, Johns Hopkins Univ. Applied Physics Lab., Laurel, MD.

Second Workshop on Harsh-Environment Mass Spectrometry, 18-21 March 2001, St. Petersburg, Florida.

Time-of-flight mass spectrometers (TOF-MS) are finding many uses in field-portable and remote sampling applications due to their inherent simplicity and potential for ruggedization. Three advances improve the instrument's performance: a focusing ion extraction source, a flexible circuit-board reflectron, and a low-noise channelplate detector assembly. The author discusses these improvements in design, along with a new configuration of an arrayed TOF analyzer for rapid parallel processing and high volume throughput.

<http://cot.marine.usf.edu/hems/workshop/2ndworkshop/presentation.htm>

#### A Miniaturized Cylindrical Ion Trap Mass Spectrometer

Patterson, Garth E.; R. Graham Cooks, Purdue Univ., West Lafayette, IN.

Second Workshop on Harsh-Environment Mass Spectrometry, 18-21 March 2001, St. Petersburg, Florida.

Miniaturization of an ion trap mass spectrometer is made possible only in part by the miniaturization of the mass analyzer itself. Fundamental trapping parameters allow for the cylindrical ion trap to arguably be the simplest mass spectrometer to miniaturize. The applied voltage needed to create a trapping field and eject the ion population is proportional to the size of the ion trap, which means the rf power supply can be miniaturized along with the mass analyzer. Because the number of collisions experienced by a given ion is minimized (as the ion's excursion is necessarily smaller), the ion trap can operate at a higher pressure, alleviating the need for a powerful vacuum pump. The two largest components of an ion trap mass spectrometer, the vacuum system and the rf power supply, can be miniaturized by using a smaller cylindrical ion trap. The authors have helped construct a miniaturized mass spectrometer based on cylindrical ion trap technology. This system has a smaller vacuum system and a much smaller rf power supply, taking advantage of the factors mentioned above.

<http://cot.marine.usf.edu/hems/workshop/2ndworkshop/presentation.htm>

#### Miniaturized GC/MS Instrumentation for in Situ Measurements: Micro Gas Chromatography Coupled with Miniature Quadrupole Array and Paul Ion Trap Mass Spectrometers

Holland, P.M. (Thorleaf Research, Inc.); Ara Chutjian, M. Darrach, O. Orient (Jet Propulsion Lab).

In Situ Instruments Workshop, 11-13 June 2002, Pasadena, California. NASA, Jet Propulsion Laboratory, Center for In-Situ Exploration and Sample Return.

The authors are developing miniaturized GC/MS instrumentation that combines chemical separations by gas chromatography (GC) with mass spectrometry (MS) to provide positive identification of chemical compounds in complex mixtures of gases, such as those found in the International Space Station's cabin atmosphere. The designs use micro gas chromatography components coupled with either a miniature quadrupole mass spectrometer array (QMSA) or a compact, high-resolution Paul ion trap. Key design issues include high sensitivity, good MS resolution (0.5 amu FWHM or better), low power, robustness,

low GC flow rates to minimize vacuum-pumping requirements, and the use of a modular approach to adapt to different environments. This work has been carried out in part at the Jet Propulsion Laboratory/California Institute of Technology with support from NASA.

#### Miniaturized Spectrometer for Stand-Off Chemical Detection

Henning, P.F. (Foster-Miller, Inc.); S. Chadha; R. Damren; R.C. Rowe; C. Stevenson; L.E. Curtiss; T.G. DiGiuseppe.

Instrumentation for Air Pollution and Global Atmospheric Monitoring. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4574, p 37-43, 2002

Foster-Miller has successfully designed and demonstrated a high spectral throughput monolithic wedge spectrometer capable of providing early, stand-off detection of chemical threats. Recent breakthrough innovations in IR source technologies, high D\* multispectral array detectors, and IR waveguide materials have supported the development of a robust, miniature, monolithic infrared spectrometer. The high resolution spectrometer has been demonstrated operating in the 8- to 12-micron region for chemical agent detection. This paper discusses the feasibility of adapting the wedge spectrometer to operate as an upward-looking ground sensor for stand-off chemical detection.

#### Monitoring Biodegradation of Creosote in Soils Using Radiolabels, Toxicity Tests, and Chemical Analysis

Phillips, Theresa M. (GRACE Bioremediation Technologies, Mississauga, Ontario, Canada); A.G. Seech; D. Liu; H. Lee; J.T. Trevors.

Environmental Toxicology, Vol 15 No 2, p 99-106, 2000

The researchers investigated the ability of soil microorganisms to become acclimatized to and to degrade creosote and radiolabeled phenanthrene in spiked soil samples, and also assessed the amount of radiolabeled carbon dioxide that evolved in soil samples kept under various moisture, temperature, and concentrations of phosphorus and nitrogen.

#### Monitoring of Environmental Changes Caused by Hard-Coal Mining

Fischer, Christian (Technische Univ. Clausthal), Wolfgang Busch.

Remote Sensing for Environmental Monitoring, GIS Applications, and Geology. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4545, p 64-72, 2002

Mining activities can cause changes of the topographic and hydrologic situation that can be detected and monitored by remote sensing. This paper describes a project to estimate dynamic changes in the surface (i.e., subsidence), ground water, and vegetation. The ground-water recharge rate and isobars of the ground-water table were calculated in detail repeatedly, starting in 1993 and aiming for 2004. Because of the great size of the area to be monitored, airborne surveys were done in August 1998 and 2000 with the HyMap imaging spectrometer, with interim monitoring results of terrestrial areas and measured LAI data as references. With spectral unmixing routines, specific information on selected land-use classes was obtained and areas affected by water logging could be identified.

#### Monitoring of Volatile Organic Components Associated with Waste Disposal Activities and Gas Pipeline Leaks with a Man-Portable Mid-Infrared DIAL

Degtiarev, Egor V. (LaSen, Inc.), A.R. Geiger; R.D. Richmond (Air Force Research Lab.).

Laser Radar: Ranging and Atmospheric Lidar Techniques III. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4546, p 74-81, 2002

LaSen's first-generation ground-based sensor (Lidar I) measures 0.19 cubic meters and weighs 55 kg. The unit was field-tested in 1991 by measuring methane levels at rural dumpsites and monitoring emissions from contaminated soil at a diesel fuel spill site. LaSen developed a compact tunable mid-infrared laser source based on an intracavity optical parametric oscillator. The laser source delivers up to 1.3 mJ of mid-infrared energy per pulse and is angularly tuned in the 3-5 micrometers band through a servo-controlled loop. A piezo-driven tuner for fast switching between on and off lines is available as an option.

#### Monitoring the Size and Metabolic Activity of the Bacterial Community During Biostimulation of Fuel-Contaminated Soil Using Competitive PCR and RT-PCR

Ka, J.O.; Z. Yu; W.W. Mohn, Univ. of British Columbia, Vancouver, BC, Canada.  
Microbial Ecology, Vol 42 No 3, p 267-273, 2001

A method developed to monitor the density and metabolic activity of the total bacterial community in soil was applied to microcosms of Arctic soil after addition of nitrogen and phosphorus to stimulate biodegradation of petroleum contaminants. The total petroleum hydrocarbon level in the soil fell from 850 to 360 µg/g of soil over the 29 days of incubation. DNA and RNA were extracted from soil using a bead beating method, purified by ammonium acetate precipitation, and assayed by competitive PCR and RT-PCR assays with universal bacterial primers. Analytical results suggest that the treatment to stimulate hydrocarbon biodegradation did not substantially change the density of the bacterial community but did increase its overall metabolic activity transiently.

#### MS for Trace Explosives Detection in Aviation Security

Chamberlain, R.T. (FAA/Wm. J. Hughes Tech. Ctr., Atlantic City, NJ), R. Lareau; K. Hanold (Syagen Technology, Inc., Tustin, CA), J. Syage; K. Linker (Sandia National Lab., Albuquerque, NM), C. Rhykerd, F. Bouchier.

Second Workshop on Harsh-Environment Mass Spectrometry, 18-21 March 2001, St. Petersburg, Florida.

The FAA has funded the development of a small dual-mode ionization mass spectrometer for the trace detection of a broad range of terrorist threats. The detector was developed by Syagen Technology, Inc. (Tustin, CA) and employs a dual ionization source for detection of explosives and chemical agents, which requires both negative and positive ion sources. The mass analyzer is a high performance ion trap, time-of-flight mass spectrometer that provides for ms-ms capability. This detector has been integrated into a personnel portal developed at Sandia National Laboratories under funding by the FAA. The key in the integration included preconcentration steps to handle large volumes of air samples. Particles and vapor have to be collected from literally several thousand liters of air volume and then introduced into a vacuum. This has to be accomplished in a time frame that is conducive to acceptable passenger flow. It was necessary to automate the process and make it simple to operate. The portal is being tested at the FAA Trace Explosives Laboratory at the Aviation Security Laboratories of the William J. Hughes Technical Center.

<http://cot.marine.usf.edu/hems/workshop/2ndworkshop/presentation.htm>

#### Multiarray Sensors for Pesticides and Toxic Metals

Xu, Hongwu (SUNY/Binghamton); M. Masila; F. Yan; O.A. Sadik.

Environmental Monitoring and Remediation Technologies. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3534, p 437-445, 1999

This paper describes the synthesis and characterization of conjugated polymers and biological components for the detection of a range of toxic substances, e.g., chlorinated phenols, s-triazine herbicides, polychlorinated biphenyls, and heavy metals. The use of o-hydroxypyridylazo metal-protein conjugates shows promise for the detection of heavy metals.

#### A Multicomponent TDL Analyzer for Open-Path Monitoring of Gaseous Atmospheric Pollutants

Chizhevskii E.G. (P.N.Lebedev Physical Institute of RAS, Moscow, Russia), O.I. Davarashvili; A.N. Khusnutdinov (Inst. of General Physics of RAS, Moscow, Russia), Ya.Ya. Ponurovskii; Yu.G. Selivanov (P.N.Lebedev Physical Institute of RAS, Moscow, Russia); E.V. Stepanov (Inst. of General Physics of RAS, Moscow, Russia), P.V. Zyrianov.

TDLS 98: 2nd International Conference on Tunable Diode Laser Spectroscopy, 6-10 July 1998, Moscow, Russia. Book of Abstracts, p 46, 1998

Some multicomponent gas detection situations requiring extra-high sensitivity, selectivity, and fast response can be solved using tunable diode lasers (TDLs). A TDL gas analyzer was developed for the detection of three gaseous pollutants with sub-ppb concentration sensitivity in open atmosphere at a stationary site. The paper contains general schematics of a TDL single-gas open-path system. Three IR detectors and three TDLs of different spectral region, one for each specific molecule, are located on the heat sink of 1-liter LN2 cryostat for separate control of the operation temperature of each laser. TDL radiation sent to open atmosphere is collimated by a two-lens objective. Radiation returned by the mirror corner is collected to the detector using the Cassegrain telescope. Up to a 600-meter to-and-from distance is available with optics used. Current pulses are used to pump TDLs and to tune their frequency due to laser crystal heating. The current pulse parameters and working temperatures are specially selected and controlled by PC for every laser for detection of the desired analytical line. For the MBE lead-salt TDL used for CO, NO, CH<sub>4</sub>, C<sub>2</sub>H<sub>4</sub>, and NH<sub>3</sub> detection, typical pulse amplitude is 0.4 to 1.5 A, pulse repetition rate is about 100 Hz, and pulse duration is up to 10 ms. Laser operation temperatures are from 80 to 130K. Stability of the analytical line position inside the pulse is defined by fluctuations of the laser temperature in the cryostat, thus the last one is controlled with 10-3K accuracy. The sensitivity of the analyzer is defined by a limit in detecting optical density variations with the acquisition system. A 50 ns, 8 bit ADC, and accumulation of the signal with fast amplitude sweeping provide 2\*10<sup>3</sup> S/N ratio. In the first stage of the project, the system was adjusted for the detection of CO, NH<sub>3</sub> and CH<sub>4</sub> in open atmosphere. The system was tested in field experiments to detect air pollution in Siberia near the Nefteugansk oil production fields in summer 1996.

#### A Multidisciplinary Approach to Screening and Characterization of Weathered Metal-Mining Waste Piles

Smith, K.S. (U.S. Geological Survey, Denver, CO); P.H. Briggs; D.L. Campbell; G.A. Desborough; R.G. Eppinger; P.L. Hageman; R.W. Leinz; G.P. Meeker; M.R. Stanton; S.J. Sutley; G.A. Swayze; D.B. Yager.

Earth System Processes -- Global Meeting, 24-28 June 2001, Edinburgh, Scotland.  
Geological Society of America, Boulder, CO.

The U.S. Geological Survey Mine Waste Characterization Project has taken a multidisciplinary approach to assemble, develop, and refine methods and tools for characterizing and screening weathered solid mine wastes. During the development of an integrated "tool kit" for the rapid and effective characterization of mine site effects, detailed studies were conducted at eight sites, representing both igneous-hosted and carbonate-hosted polymetallic sulfide deposits. The carbonate-hosted sites enabled an evaluation of the possible mitigating effects of carbonate minerals. Two of the sites located in a drier climate allowed scientists to examine the influence of climate on mine-waste weathering processes.

Findings from this work will assist land managers, industry, and regulatory agencies in ranking and prioritizing mine-waste piles for remediation.

#### Multi-ImmunoSensors Based on Electrolyte-Insulator-Semiconductor Structures for Determination of Some Herbicides

Starodub, N.F. (A.V. Palladin Inst. of Biochemistry); V.M. Starodub; V.E. Krivenchuk; V.F. Shapovalenko.

Advanced Environmental Sensing Technology II. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4576, p 56-62, 2002

A new type of multi-immune sensor for the determination of herbicides is based on electrolyte-insulator-semiconductor structures. Specific antibodies were immobilized on nitrocellulose disks, which were placed in measuring cells. The analysis was fulfilled by sequential saturation of antibodies, left unbound after their exposure to an herbicide in a sample. A horse radish peroxidase label for the multi-immune sensor achieved sensitivities of about 5 and 1.25 µg/L for simazine and 2,4-D, respectively. With a (beta)-glucose oxidase label, the sensitivity of herbicide analysis increased approximately 5 times.

#### Multisensor Analyzer Detector (MSAD) for Low Cost Chemical and Aerosol Detection and Pattern Fusion

Swanson, D.C. (Pennsylvania State Univ.); D.W. Merdes; D.B. Lysak; R.C. Curtis; D.C. Lang; A.F. Mazzara; N.C. Nicholas.

Sensors, and Command, Control, Communications, and Intelligence (C3I) Technologies for Homeland Defense and Law Enforcement. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4708, p 226-232, 2002

A Multisensor Analyzer Detector (MSAD) is being developed as a low-cost point detection chemical and biological sensor system designed around an information fusion inference engine that allows additional sensors to be included in the detection process. The MSAD concept is based on probable cause detection of hazardous chemical vapors and aerosols of either chemical or biological composition using a small portable unit containing an embedded computer system and several integrated sensors with complementary capabilities. The system includes a surface-enhanced Raman spectroscopy (SERS) sensor of chemical vapors and a detector of respirable aerosols based on Fraunhofer diffraction. Sensors employing ion mobility spectrometry (IMS), surface acoustic wave (SAW) detection, flame photometric detection (FPD), and other principles also are candidates for integration into the device.

#### Multisensor Data Integration and Adaptive Sampling Strategies for an Autonomous Underwater Mass Spectrometer

Camilli, Richard; Harold F. Hemond, Massachusetts Inst. of Technology.

The 3rd Harsh-Environment Mass Spectrometry Workshop, 25-28 March 2002 Pasadena, California.

Scientists are examining the use of real-time chemical data from an underwater mass spectrometer operating onboard an autonomous underwater vehicle (AUV), in concert with data from other sensors commonly used on these robots, for pattern recognition and effective adaptive sampling. This strategy is implicitly useful for a host of applications, including concurrent and feature-based mapping, improving acoustic and magnetic sensor data interpretation, direction of chemotactic searches, and adaptive control of mass spectrometer scanning. This paper describes a pattern recognition system within a layered control architecture for use with the NEREUS underwater mass spectrometer and the Odyssey autonomous underwater vehicle.

<http://cot.marine.usf.edu/hems/workshop/3rdworkshop/program.htm>



### New Promising Multipass Systems for FTIR and TDL Spectroscopy

Chernin, S.M., General Physics Inst., Moscow, Russia.

TDLS 98: 2nd International Conference on Tunable Diode Laser Spectroscopy, 6-10 July 1998, Moscow, Russia. Book of Abstracts, p 35, 1998

New long-path mirror systems have been developed for high-resolution spectroscopy. As compared to the classical White system, the new ones involve new design features as well as improved optical and performance characteristics. The V-shaped mirror system has the highest f number ( $f/3.7$ ) among other multipass systems due to nontraditional choice of a base length equal to  $1.5 f$  between opposite mirrors. The V-shaped six-pass system consists of two mirror-symmetrical three-pass systems of forward and reverse passages, which unfold into a Z-shaped Czerny scheme. This optical system served as a basis for the cells designed for FTIR and TDL spectroscopy. The total absorption length was 1.2m (0.5 l) in the cell for FTIR and 3m (6.6 l) in the device for TDL spectroscopy. The V-shaped system has practically no aberrations.

### New Remote Sensing Concepts for Environmental Monitoring

Ehlers, Manfred (Univ. Vechta); R. Janowsky; M. Gaehler.

Remote Sensing for Environmental Monitoring, GIS Applications, and Geology. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4545, p 1-12, 2002

This paper offers a brief overview of different methods of remote sensing for global, regional, and local environmental monitoring. New technologies such as global positioning system (GPS), digital photogrammetry, and multi-source satellite remote sensing are creating data at high spatial, spectral, and temporal resolution. Geographic Information Systems (GIS) technologies allow the efficient storage and management of spatial datasets in digital formats. Multispectral satellite scanners in the visible and near infrared domains of the electromagnetic spectrum record solar radiation reflected from the earth's surface, and these data provide information on geomorphology, soils, surface waters, river networks, and vegetation type, distribution and condition. The authors also comment on active microwave radar systems, satellite remote sensing systems, and digital airborne cameras.

### New Spectrascan™ Vegetation Type, Distribution and Condition; Open Path Monitor: Bovar Western Research Launches New Spectrascan™ Open Path Monitor Garden State Environet, 28 Jun 1995

BOVAR Western Research (San Antonio, TX) reports the launch of the SpectraScan™ tunable diode laser-based system for perimeter monitoring of toxic and hazardous gases. Developed as a joint industry project by Spectrum Diagnostix with selected members of the Petroleum Environmental Research Forum (PERF), SpectraScan™ is an accurate spectroscopic technique for measuring minute concentrations of gases such as hydrogen fluoride and hydrogen sulfide in refining and industrial applications. SpectraScan™ allows economical, high precision measurement of single or multiple gas species using near infrared lasers. The product's accuracy is attributable to its tunable diode laser, which is tuned to specific wavelengths, allowing for sensitive measurement of gases along an open path up to 200 meters. As each laser wavelength is highly specific to the gas being monitored, there is no interference from particulate or other gas species. Detection and measurement are accurate and interference-free. BOVAR Western Research manufactures and assembles its analyzers and systems in Calgary, Alberta; Houston; and Hattersheim, Germany. SpectraScan™ is the trade name of Spectrum Diagnostix, Incorporated (SDx) of Andover, Mass. Contact: Len Edwards, BOVAR Western Research, 800-661-9198 or 403-235-8406.

New Widely Tunable Mid-IR Lasers and Their Use in Molecular Spectroscopy  
Jeffers, James (Ekips Technologies, Inc.), P.J. McCann, K. Namjou, C. Roller; Z. Debebe (Univ. of Oklahoma), J. Grego.  
Instrumentation for Air Pollution and Global Atmospheric Monitoring. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4574, p 201-207, 2002

This paper presents results from detailed measurements of IV-VI diode laser emission obtained using an automated Fourier transform infrared (FTIR) spectroscopic testing system. Single mode emission wavelengths were determined for different combinations of heatsink temperature and injection current. These data were applied to molecular spectroscopy experiments to modulate laser emission wavelength by either current or temperature tuning. Current tuning over narrow spectral regions (up to  $3\text{ cm}^{-1}$ ) allowed detection of various small to medium sized molecules (e.g., carbon disulfide, ammonium hydroxide, and benzene), but failed to detect larger molecules such as toluene. Temperature-tuning a IV-VI laser over at least  $50\text{ cm}^{-1}$  can extend the use of mid-infrared laser spectroscopy to measurement of large molecules that do not have resolvable ro-vibrational structure.

Non-Invasive Imaging of Flow and Transport in Soil Monoliths Using Magneto-Electrical Resistivity Tomography: Concept and Instrumentation  
Kemna, A.; E. Zimmermann; W. Glaas; K.-H. Herrmann.  
Geophysical Research Abstracts, Vol 4, 27th General Assembly, European Geophysical Society [Abstracts] 2002

Magneto-electrical resistivity tomography represents a new and promising approach in non-invasive measurement techniques capable of imaging and characterizing water flow and solute transport in soils. The technique is based on the measurement of magnetic field distributions due to a variety of electric current patterns impressed into the soil. The bulk electrical conductivity distribution within the soil can be imaged with high spatial resolution by means of adequate tomographic inversion algorithms. In contrast to standard electrical resistivity tomography, magnetic sensors do not require galvanic coupling and hence enable flexible and efficient data acquisition around a given soil monolith. This paper presents the concept and an advanced instrumental setup for magneto-electrical resistivity tomography as applied to soil column experiments at both laboratory and lysimeter scale. Magnetic data acquisition is based on anisotropic magneto-resistive sensors, which could be electronically implemented such as to provide sufficient sensitivity to detect the relatively small magnetic fields associated with the method. Preliminary investigations indicate that the developed system meets the requirements for high-resolution imaging of flow and transport processes in soil monoliths.

Non-Invasive Methods for Quantitative Imaging of Solute Transport in Porous Media at Different Scales  
Kemna, A.; J. Vanderborght; A. Pohlmeier; H. Vereecken.  
First Workshop on Mathematical Modelling of Environmental Problems, 17-21 June 2002, Romanian Academy, Institute of Mathematical Statistics and Applied Mathematics, Bucharest [Abstracts].

Magnetic Resonance Imaging (MRI) and Electrical Impedance Tomography (EIT) are non-invasive measurement techniques capable of imaging and monitoring water flow and transport processes quantitatively at different spatial scales. MRI is increasingly being used in controlled soil column experiments to directly image fluid motion and dispersion. Results from recent experiments on calibrated porous media in particular indicate that the overall effective dispersion is dominated by larger-scale structural inhomogeneities rather than local dispersive effects. EIT images electrical conduction and polarization parameters, which are closely related to flow and transport properties. The underlying measurement principle is easy to implement at various scales, and is applicable in both

lysimeter and field studies. EIT results depend on certain a-priori assumptions on the medium under investigation, and the authors illustrate the capabilities and limitations of the method with the results from a synthetic model example and a field tracer experiment conducted in a heterogeneous aquifer. Advances in the area of non-invasive sensing include a new Magneto-Electrical Resistivity Imaging Technique (MERIT), representing a combination of EIT and the magnetometric resistivity method mainly used in exploration geophysics. By exploiting both electric and magnetic field information, MERIT is expected to yield improved image resolution compared to standard EIT.

#### A Novel Voltammetric In-Situ Profiling System for Continuous Real-Time Monitoring of Trace Elements in Natural Waters

Tercier, Mary-Lou (Univ. of Geneva, Geneva, Switzerland); Jacques Buffle; Flavio Graziottin. *Electroanalysis*, Vol 10 No 6, p 355-363, May 1998

This article describes a novel voltammetric in situ profiling system (VIP System) for continuous, real-time monitoring of trace elements in fresh and seawater down to a depth of 500 meters. The heart of the submersible voltammetric probe is a Hg-plated Ir-based microsensor covered with an antifouling gel membrane. This gel-integrated microsensor allows direct voltammetric measurements of trace metals in complex media without physical and chemical interferences of the test solution. The system has been applied to in situ trace metal monitoring in oxygen-saturated seawater, as well as in situ profiling of MnII in anoxic lake water. The performance of the VIP System was robust and reliable, achieving in situ measurements of mobile fraction of trace metals down to concentration levels as low as ~5 ppt.

#### Odor Sensor using Plasma-Polymerized-Film-Coated QCM for Environmental Monitoring

Nanto, Hidehito (Kanazawa Inst. of Technology), Y. Hamaguchi, S. Sanada, K. Nobuyama; T. Matsumoto (Natl. Inst. of Advanced Industrial Science and Technology), K. Tanabe, S. Kurosawa. *Advanced Environmental Sensing Technology II. Proceedings of SPIE - The International Society for Optical Engineering*, Vol 4576, p 237-243, 2002

In developing a sensor system for environmental monitoring, chemical sensors using quartz crystal microbalance (QCM) coated with acrylate-film with different functional groups have been combined with styrene-film as a molecular recognition membrane. The sensors were prepared using a plasma-polymerized chemical vapor deposition method. Sensor response for various gases depends on the functional group of the sensor's molecular recognition membrane. The styrene film-coated sensor exhibited no selectivity for specific gas and responded to various gases. In conjunction with principal component analysis, the styrene-film coated sensor can be used to identify gases in environmental monitoring.

#### Oleoresin Chemistry and Spectral Reflectance in "Stressed" Lodgepole and White Bark Pine, Mammoth Mountain, California

Hickey, James C.; Richard W. Birnie; Meixun Zhao.

AVIRIS Airborne Geoscience Workshop Proceedings 2001. Jet Propulsion Laboratory, California Inst. of Technology. 10 pp, 2001

Alterations in the soil/sediment geochemical environment can result in foliar chemical changes that are detectable via remote sensing, e.g., monitoring chlorophyll reflectance/fluorescence and equivalent water thickness indices as indicators of drought-induced plant stress. Principal components analysis (PCA) of hyperspectral data has been used to identify absorption feature patterns obtained from vegetated areas with discrete bedrock geology or mineralization as the substrate. This paper describes an investigation to elucidate the connection between changing geochemical substrates (high CO<sub>2</sub> in soil

gas), resultant changes in conifer biochemistry (i.e., monoterpenes in oleoresin and other coincidentally responding constituents), and any associated alteration of the plant's reflectance curve. Predicting a change in monoterpene/oleoresin chemistry and in turn the geochemical substrate, using either field spectroscopy or hyperspectral imagery, is the ultimate goal of the research behind this project.  
[http://popo.jpl.nasa.gov/docs/workshops/01\\_docs/toc.html](http://popo.jpl.nasa.gov/docs/workshops/01_docs/toc.html)

#### On-Line Microbial Biosensing and Fingerprinting of Water Pollutants

Horsburgh, A.M. (Univ. of Aberdeen, Aberdeen, Scotland, UK), D.P. Mardlin, N.L. Turner; R. Henkler (ICI Paints, Wexham Road, Slough, UK); N. Strachan (University of Aberdeen, Aberdeen, Scotland, UK), L.A. Glover, G.I. Paton, K. Killhama.  
Biosensors and Bioelectronics, Vol 17 No 6-7, p 495-501, 2002

This paper reports the use of novel slow release biosensor delivery for on-line monitoring instrumentation, with environmentally relevant bacteria for both simple toxicity testing and more complex toxicity fingerprinting of industrial effluents. Using bioluminescence-based biosensors, the on-line toxicity test proved to be as sensitive and reliable as the corresponding batch test, with comparable contaminant EC50 values from both methods. The slow release of biosensors immobilized in a polyvinyl alcohol (PVA) matrix greatly improved biosensor delivery, did not affect the sensitivity of toxicity testing, and showed great potential for incorporation in on-line monitoring instrumentation.

#### Optical-Fiber-Based Groundwater Sensor for Monitoring Landfill Sites

Spencer, J.W. (Univ. of Liverpool), S.R. Smith, G.R. Jones; E.M. Dean (British Nuclear Fuels plc), J.C. Simpson.  
Chemical, Biochemical and Environmental Fiber Sensors IX. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3105, p 275-282, 1997

This paper describes an optical fiber-based sensor for monitoring the concentration of particulate material that may be entrained in ground water. The sensing system uses white light from a multi-wavelength spectral source transmitted through a 200-micrometer diameter multimode fiber to a sensing head. The infrared portion of the light acts as a reference while the visible part is transmitted through a sampling area and is reflected back in to a receiving fiber. A dual epitaxial diode detects the reference and modulated spectra. Discrimination between air and water is possible through Mie scattering because of differences in the absorption spectra and refractive indices, and between water with and without particulates.

#### Optical Fiber Sensors for the Distributed Measurement of Hydrocarbons

Burck, Jochen; Elke Sensfelder, Forschungszentrum Karlsruhe, Germany.  
Chemical, Biochemical, and Environmental Fiber Sensors X. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3540, p 98-109, 1999

A chemically sensitive polymer-clad silica fiber adapted to different optical time domain reflectometer (OTDR) setups provides the basis for truly distributed sensing systems for nonpolar hydrocarbons. OTDR measurements allow to investigators to locate and detect chemicals by measuring time delay between short light pulses entering the fiber and discrete changes in the backscatter signals caused by chemical effects in the fiber cladding. This paper offers the initial data on the distributed sensing of chlorinated hydrocarbons (CHCs) with a commercially available mini-OTDR adapted to a sensing fiber of nearly one kilometer length. A laser diode emitting at the 850-nm telecommunication wavelength was applied to locate the CHCs by analyzing the step drop (light loss) in the backscatter signal caused by refractive index changes in the silicone cladding induced by analyte enrichment.

#### Optical Multiple-Analyte Immunosensor for Water Pollution Control

Barzen, Claudia (Inst. of Physical and Theoretical Chemistry, Univ. of Tuebingen, Tuebingen, Germany); Andreas Brecht; Guenter Gauglitz.

Biosensors and Bioelectronics, Vol 17 No 4, p 289-295, Apr 2002

A prototype of a portable optical immunosensor (the 'river analyzer') has been developed that can be applied for the monitoring of surface water quality. Antibodies carrying a fluorescent label are used for the specific recognition of pollutants such as pesticides. The transduction principle is based on total internal reflection fluorescence. The river analyzer can detect at least three analytes simultaneously in one sample, and automated test cycles and fluid handling enable unattended measuring.

#### Optical System-on-a-Chip for Chemical and Biochemical Sensing: the Chemistry

Campbell, Daniel P. (Georgia Tech Research Inst.), J.L. Moore, J.M. Cobb, N.F. Hartman; B.H. Schneider (Photonic Sensor Systems, Inc.), M.G. Venugopal.

Chemical, Biochemical, and Environmental Fiber Sensors X.

Proceedings of SPIE - The International Society for Optical Engineering, Vol 3540, p 153-161, 1999

Planar waveguides have evanescent fields sensitive to index of refraction changes in the volume immediately above the waveguide surface. Optically combining one guided sensing beam with a reference beam in an interferometric configuration generates measurable signals. Applying a chemically selective film over the sensing arm of the interferometer provides the basis for a chemical sensor. The integrated optic waveguide platform discussed in this paper consists of thirteen interferometers on a 1 x 2-cm glass substrate. A different sensing film deposited on each channel allows for multiple analyte sensing, interferant cancellation, patterned outputs for analyte identification, or extended dynamic range. Sensitivities range from the low ppm to low ppb for both vapor and aqueous applications, 0.01 pH units and ng/mL for biologicals.

#### Optimization of Composite Polymer Gas Sensor Arrays for Single-Analyte Multiple-Interferent Applications

Wilson, Denise M., Univ. of Washington.

Advanced Environmental Sensing Technology II. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4576, p 207-214, 2002

This paper presents results from optimizing an array of composite polymer gas sensors for sensing one of five analytes (acetone, hexane, thf, toluene, and ethanol) in the presence of up to four interferents. The optimized array consists of a heterogeneous array of up to ten points (unlike sensors) in multi-dimensional sensor space. The optimization techniques presented here are linear, since the composite polymer sensors in their useful (low concentration) operating range exhibit linear and additive response characteristics. The optimization of these arrays produces maximum separability between analytes, demonstrating the trade-off between the addition of both information and variability induced by increasing the size of the heterogeneous array.

#### Optimized Configurations for Mid-Infrared Fiber Optic Sensors in the Marine Environment

Kraft, Martin (Vienna Univ. of Technology), M. Jakusch, B. Mizaikoff; A. Katzir (Tel Aviv Univ.).

Infrared Optical Fibers and Their Applications. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3849, p 28-36, 1999

A portable sensor system for marine real-time, in situ monitoring of chlorinated hydrocarbons in seawater consists of a robust, miniaturized FTIR spectrometer in a sealed aluminum pressure vessel with a suitable fiber-optic sensor head attached to one of the container end plates. The signal generation is based on fiber evanescent wave spectroscopy, an application of the internal reflection spectroscopy principle. A hydrophobic polymer coating the sensor head enriches hydrophobic analytes from the seawater matrix and protects the fibers from corrosion by aggressive seawater constituents.

#### Optimized Sensitive Coatings for MIR Fiber Optic Sensors

Jakusch, M. (Vienna Univ. of Technology), B. Mizaikoff, R.A. Kellner; A. Katzir (Tel Aviv Univ.). Chemical, Biochemical and Environmental Fiber Sensors IX. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3105, p 283-288, 1997

The researchers have investigated novel coating materials for MIR fiber-optic sensors to assess the possibilities and limitations associated with introducing materials of higher molecular complexity as coatings. In the study, poly(acrylonitrile-co-butadiene) and poly(styrene-co-butadiene) showed increased sorption coefficients for substances such as chlorinated phenols and anilines together with only moderately narrowed spectral windows.

#### Passive Sampling Devices (PSDs) as Biological Surrogates for Estimating the Bioavailability of Organic Chemicals in Soil

Wells, Jason B.; R.P. Lanno, Dept. of Zoology, Oklahoma State Univ., Stillwater.

Environmental Toxicology and Risk Assessment: Science, Policy, and Standardization--Implications for Environmental Decisions, 10-12 April 2000, Toronto, Ont., Canada. American Society for Testing and Materials, Reston, VA. ASTM Special Technical Publication No 1403. p 253-270, 2001

Organic chemical exposure in soil toxicity tests and in ecological risk assessment of terrestrial systems is usually expressed as the total chemical measured. Possible alternatives to total chemical measures of organic chemical bioavailability and exposure include body residues in test organisms, soil extraction with selective solvents, and passive sampling devices (PSDs) as biological surrogates. Semipermeable membrane devices (SPMDs) offer potential as a biological surrogate in soil systems. Solid-phase microextraction (SPME) fibers are a rapid and sensitive means for detecting PAHs in soil and have the advantage of not requiring solvent extraction of soil. The authors undertook a study to compare chemical uptake and residues in earthworms, SPMDs, and SPMEs exposed in artificial soil spiked with phenanthrene (PHE). Bioavailable PHE, as assessed by mortality and PHE body residues, varied dramatically with soil organic matter content. Both SPMEs and SPMDs could discriminate differences in PHE availability between treatments, but PHE levels measured using SPMEs were more precise and allowed discrimination between toxic and non-toxic levels of PHE. PHE levels in SPMDs were too variable for use as a predictive tool.

#### Passive Standoff Detection of Surface Contaminants: Modeling the Spectral Radiance

Theriault, Jean-Marc (Defence Research Establishment Valcartier); J.O. Jensen (U.S. Army Soldier and Biological Chemical Command), A.C. Samuels; A. Ben-David (SAIC); C.M. Gittins (Physical Sciences Inc.), W.J. Marinelli.

Instrumentation for Air Pollution and Global Atmospheric Monitoring. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4574, p 26-36, 2002

A study to estimate the spectral radiance of surface contaminants has been undertaken to address issues relevant to the passive standoff detection of such contaminants. SF96 and Krylon 41325 were chosen as contaminant simulants, and their contamination of four different surfaces (aluminum, grass, soil, and

plywood) was analyzed. Measurements of spectral radiance with the CATSI system were compared with the best-fit spectra derived from a first order model of reflectance. The experimental results agreed well with the model best fits for Krylon on aluminum and grass samples, though not for Krylon on soil and SF96 on plywood.

Performance Evaluation of the Westinghouse Science and Technology Center's Prompt Gamma Neutron Activation Analysis Prototype for Verification Assay of Mercury in Mixed Waste  
McIlwain, Michael E., Idaho National Engineering and Environmental Lab., Idaho Falls, ID.  
Report No: INEEL/EXT-02-00011. 14 pp, Jan 2002

The ability of a prototype prompt gamma neutron activation analysis (PGNAA) instrument, developed by Westinghouse Science and Technology Center, to measure the mercury content of inorganic sludge was evaluated. Eight samples, containing mercury concentrations of 0 to 117 parts per million (ppm), were selected from the inventory of Rocky Flats' inorganic sludge. Two separate test protocols were developed, one based on blind assay of the test samples and the other a contingency in case the instrument failed to detect mercury in any test samples. The PGNAA instrument initially failed to blind assay the test samples. Westinghouse was permitted to alter the instrument's operation until correct assays were obtained. Following these modifications, the PGNAA instrument functioned within its anticipated performance limits. It was able to reproducibly detect mercury concentrations greater than its lower limit of detection (60 ppm of mercury), and gave no false positive detections for concentrations less than 60 ppm. The PGNAA instrument is not ready for routine verification assay of sludge waste forms. It requires additional optimization and testing on other waste forms; however, the assay results support continued development of the instrument. Its operation should be modified to better assay waste, and it should be tested on additional characterized waste forms.  
<http://tmfa.inel.gov/Documents/technical.asp>

Photon-Counting Spectrometer for Elemental Analysis Using LIBS  
Taylor, David (Radiation Monitoring Devices, Inc.); Richard Myers; Arieh Karger.  
In Situ Instruments Workshop, 11-13 June 2002, Pasadena, California. NASA, Jet Propulsion Laboratory, Center for In-Situ Exploration and Sample Return.

Avalanche photodiode (APD) arrays are being applied to laser-induced breakdown spectroscopy (LIBS) for elemental analysis with standoff detection capability. This instrument benefits from the advantages common to both Geiger-mode and proportional-mode APDs, which are solid-state detectors with virtually single-photon sensitivity, higher quantum efficiency than photomultiplier tubes or intensified CCDs, and rapid sub-nanosecond response speed. The researchers have demonstrated better than part-per-million LIBS detectability utilizing the Geiger-mode APD. In a LIBS system, an APD array offers the unparalleled prospect of selecting in each channel the most appropriate temporal window for detecting the target species. In real-time detection systems, such as microfluidics-based fluorescence detection of bacterial spores, these compact, robust APD arrays promise portable hand-held instruments that utilize tight optical coupling.

Polymeric Membrane Chlorocarbon Permeabilities Determined by Membrane Introduction Mass Spectrometry (MIMS)  
Stone, Mark, Idaho National Engineering and Environmental Laboratory/Bechtel, Idaho Falls, ID.  
Second Workshop on Harsh-Environment Mass Spectrometry, 18-21 March 2001, St. Petersburg, Florida.

One promising technique for monitoring chlorocarbons is that of using semipermeable membranes to preconcentrate or semipermeably permit transport of this class of materials for analysis. This paper

presents the test results from commercially available and in-house produced membranes in a MIMS arrangement for four chlorocarbons.

<http://cot.marine.usf.edu/hems/workshop/2ndworkshop/presentation.htm>

#### A Portable Cyanide Analyzer Using Gold Wire Electrodes

Sequeira, Margaret (Univ. of New South Wales, Sydney, New South Wales, Australia); D.B. Hibbert; P.W. Alexander.

Electroanalysis, Vol 11 No 7, p 494-498, Jun 1999

A continuous flow potentiometric analyzer for cyanide incorporates multiple gold-wire electrodes. The portable apparatus comprises a low-powered peristaltic pump and a Perspex multicell incorporating six indicator and six reference electrodes connected to an eight-channel A/D converter. Real-time data can be displayed on a notebook computer. The system delivered well-defined peaks and fast response times (with peak widths <20 s) using a carrier of 0.1 M sodium hydroxide at a flow rate of 5 mL min<sup>-1</sup>.

#### Portable Double-Focus Mass Spectrograph with Multymembrane Inlet

Viktorova, Olga (A.F. Ioffe Physical Technical Inst., St. Petersburg, Russia); Viktor Kogan; Sergey Manninen.

The 3rd Harsh-Environment Mass Spectrometry Workshop, 25-28 March 2002 Pasadena, California.

A portable mass spectrometer has been designed for direct, permanent, autonomous, in situ analysis of a mixture's composition in real time. Small size and weight, low energy consumption, and high sensitivity to organic compounds render it suitable for environmental investigation. A simple design and small permanent magnets that require no power at all make the static mass spectrometer attractive for miniaturization. Mass spectrography mode gives the best results because it can monitor for several compounds simultaneously. A number of volatile and semivolatile organic compounds have a high permeability through the silicone membrane in comparison with the nature matrix (air, water) permeability. The multimembrane inlet increases the sensitivity of the mass spectrometer for organic impurities in air by many times more. The Double-Focus Mass Spectrograph with Multymembrane Inlet is a real prototype of the portable instrument.

<http://cot.marine.usf.edu/hems/workshop/3rdworkshop/program.htm>

#### A Portable Fiber-Optic Pesticide Biosensor Based on Immobilized Cholinesterase and Sol Gel Entrapped Bromocresol Purple for In-Field Use

Andreou, Vangelis G.; Yannis D. Clonis, Agricultural Univ. of Athens, Athens, Greece.

Biosensors and Bioelectronics, Vol 17 No 1-2, p 61-69, Jan 2002

This paper reports on the development of a fiber-optic biosensor for the detection and determination of the pesticides carbaryl and dichlorvos. The sensing bioactive material was arranged like a three-layer sandwich. The enzyme cholinesterase was immobilized on the outer layer, which consisted of a hydrophilic modified polyvinylidene fluoride membrane. The membrane was in contact with an intermediate sol-gel layer that incorporated bromocresol purple, deposited on an inner glass disk. The sensor operated in a static mode at room temperature, and the rate of the inhibited reaction served as an analytical signal. The method was successfully applied to the detection and determination of carbaryl and dichlorvos in real water samples, without sample preparation steps and with 94.9% accuracy. Without enzyme regeneration steps, the sensor lifetime was 3 weeks, with a 30% activity reduction.

#### Portable Gamma-Ray Transmission System for Identification of Chemical Agents



Roney, Tim J. (National Engineering and Environmental Lab.), T.A. White, R.J. Pink; M. Smith (Idaho State Univ.), W.F. Jones.  
Penetrating Radiation Systems and Applications. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3769, p 11-23, 1999

A field-portable instrument has been developed for the purpose of classifying and identifying chemical agents within munitions by measurement of the linear attenuation property of the agent. The instrument allows for several degrees of freedom to accommodate multiple data acquisition protocols, including tomographic imaging. A variety of algorithms have been investigated, including single-ray transmission to complete 2-D computed tomography using a collimated isotopic source. Recent results from laboratory and field studies indicate that gamma ray measurements can provide identification of chemical agents in reasonable time frames.

#### The Portable Horiba-Kore Mass Spectrometer MS-200

Nuber, Frank (Kore Technology, Ltd., Cambridge, England); S. Mullock; W.R. Gentry; C. Corlett.  
Second Workshop on Harsh-Environment Mass Spectrometry, 18-21 March 2001, St. Petersburg, Florida.

The MS-200 is a battery-operated, portable membrane inlet, time-of-flight mass spectrometer. This technique allows semi-continuous real time in situ analysis of VOCs in gaseous samples. The paper describes some of the features and design considerations, working principles of the inlet system, the mixture analysis software, and limitations of the technology.

<http://cot.marine.usf.edu/hems/workshop/2ndworkshop/presentation.htm>

#### Portable Methane Analyzer Based on Tuned Near IR Diode Laser for Measurements in Open Atmosphere

Berezin, A. (General Physics Inst., Moscow, Russia); S.Chernin; O.Ershov; V.Kutnyak; A. Nadezhdinskii.

TDLS 98: 2nd International Conference on Tunable Diode Laser Spectroscopy, 6-10 July 1998, Moscow, Russia. Book of Abstracts, p 33, 1998

Near-infrared (near-IR) diode laser-based instruments for measuring gas concentration have an essential advantage over mid-IR instruments: they do not require cooling equipment. The main disadvantage of the near-IR spectral range is that for most molecules of interest, only overtones and combination bands are located in this range, which have much less absorption in comparison with fundamental bands in mid IR. The combination of a multipass cell with optical path length up to 100 m, low noise electronic unit, original signal processing, and the gas concentration calculation procedure used in the portable methane analyzer allows this disadvantage to be overcome and confers very high sensitivity in the near-IR range. The gas analyzer is intended for continuous automatic gas concentration measurements with data stored in computer memory. The measurements could be done in the open atmosphere as well as for gas mixture samples in a closed cell. The device made for methane concentration measurements can be converted easily for another gas by changing the diode laser. The Chernin four objective mirrors multipass cell (base length 0.5 m, diameter 0.15 m) tuned to 156 passes is an analytical optical part of the analyzer. Gas concentration measurements were performed with the help of a reference channel, including a closed cell of pure methane. The laser was able to radiate in two opposite directions through the analytic (multipass) cell and reference cell. Photodetectors' signals at the outputs of both channels were used for the normalization and gas concentration calculation in the analytic channel. Pulse technique was applied for absorption line detection. In this method the diode laser is driven by current pulses of sawtooth form, allowing a small portion of the spectrum to register that includes the absorption line of interest. A computer program compares the filtered photodetector

signals in both channels and calculates the gas concentration with the help of a correlation function. At a minimum measurement duration of one second, the sensitivity limit of methane detection was 50 ppb with a relative accuracy of 2%, and an estimated 100 ppb long-term sensitivity. The gas analyzer is fully automated and has functioned continuously without an operator for a period of one week.

Preliminary Results of Hydrothermal Alteration Assemblage Classification in Aurora and Bodie Mining Districts, Nevada and California, with Airborne Hyperspectral Data  
Smailbegovic, Amer; James V. Taranik; Wendy M. Calvin, Arthur Brant Laboratory for Exploration Geophysics, Univ. of Nevada, Reno.  
AVIRIS Airborne Geoscience Workshop Proceedings 2001. Jet Propulsion Laboratory, California Inst. of Technology. 8 pp, 2001

The University of Nevada at Reno has acquired both high- and low-altitude AVIRIS data of the Aurora and Bodie mining districts on opposite sides of the Nevada-California state line. Low-altitude data was acquired in July 2000, followed by high-altitude collection in October 2000. The AVIRIS coverage was targeted on the main vein system in Aurora (Prospectus and Humboldt Vein), East Brawley Peak prospect (midpoint between Aurora and Bodie) and "Bonanza Zone" (Bodie Bluff and Standard Hill) in Bodie, where the hydrothermal alteration zones appear to be the most pervasive. The ground-observations and mining/prospecting reports suggest propylitic alteration throughout the Bodie Hills, argillic and potassic alteration in Aurora and Bodie, (low-sulfidation system) and alunitic alteration (high-sulfidation system) on East Brawley Peak. The AVIRIS data allows identification of alteration zones containing dominant kaolinite, sericite (Aurora), alunite (E. Brawley Peak) and Na and Ca-montmorillonite (Bodie), which have been verified with ASD spectrometer and XRD analysis on field-collected samples. The authors present the mapping results from the high-altitude data set and an initial comparison to the low-altitude scene.

[http://popo.jpl.nasa.gov/docs/workshops/01\\_docs/toc.html](http://popo.jpl.nasa.gov/docs/workshops/01_docs/toc.html)

Quantification of a Single-Component Gas in Air with a Microhotplate Gas Sensor Using Partial Least Squares Techniques  
Ding, Junhua (Univ. of Maryland/College Park), J.T. McAvoy; R.E. Cavicchi (NIST), S. Semancik.  
Internal Standardization and Calibration Architectures for Chemical Sensors. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3856, p 162-170, 1999

The authors demonstrate that quantification of a single component gas in air with a microhotplate gas sensor operated in a temperature programmed sensing (TPS) mode made possible by using partial least squares techniques. The calculations of the PLS models are based on gas sensitivity, which is the ratio between the dynamic responses to the test gas and to air. Gas concentrations are predicted accurately for different test gases, different temperature sequences, and different metal-dosed microhotplate gas sensors.

Quantitative Analysis of Aromatic Compounds by Laser-Induced Fluorescence Spectroscopy  
Marowsky, G. (Laser-Lab. Goettingen e.V., Goettingen, Germany); F. Lewitzka; U. Buenting; M. Niederkrueger.  
Advanced Environmental and Chemical Sensing Technology. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4205, p 218-223, 2001

This paper introduces a compact fiber-optic sensor system based on laser-induced, time-resolved fluorescence emission spectroscopy. It uses a miniaturized solid-state laser operated at 266 nm as the

excitation source, and a spectrograph/image intensifier/CCD-camera for time-resolved detection of the fluorescence. The system is designed for environmental analysis applications.

#### Radiometric Linearity in Passive FTIR Spectrometry

Kroutil, R.T. (U.S. Army Edgewood Research, Development, and Engineering Ctr.); R.J.Combs; R.B. Knapp.

Internal Standardization and Calibration Architectures for Chemical Sensors. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3856, p 34-43, 1999

Passive standoff FTIR spectrometry relies on the radiance differential between a background scene and a target vapor analyte. Unlike traditional FTIR approaches controlling radiance levels within a narrow range, the passive configuration often encounters a large variance in radiance levels, which places higher demands on the passive FTIR configuration for maintaining linearity. The authors assess the radiometric linearity of a passive FTIR configuration using controlled blackbody radiance in conjunction with target samples, such as ethanol vapors.

#### Real-Time Monitoring of Chlorinated Aliphatic Compounds in Air Using Ion Mobility Spectrometry with Photoemissive Electron Sources

Walls, C.J. (North Dakota State Univ.), O.F. Swenson; G.D. Gillispie (Dakota Technologies, Inc.).

Environmental Monitoring and Remediation Technologies. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3534, p 290-298, 1999

Ion mobility spectrometry with a photoemissive electron source can be used for monitoring vapors of highly electronegative species such as chlorinated solvents and explosives. This paper describes the methodology and the response characteristics of a developed instrument, and summarizes the relevant ion-molecule reactions.

#### Real-Time REMPI Detection of Benzene and Toluene: a Progress Report

Gillispie, Gregory D. (Dakota Technologies, Inc.), J.L. Klingfus; S. McCormack (Brown Univ.).

Solid State Lasers IX. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3929, p 208-215, 2000

This paper focuses on real-time detection of benzene and toluene via resonance-enhanced multi-photon ionization (REMPI). The 266.0 nm 4th harmonic wavelength from a Nd:YAG laser falls within the first UV absorption system of single ring benzenoid compounds, but overlap with the structured absorbance bands exhibited by benzene and toluene is poor. Tunable solid-state laser options under consideration include Yb:YAG and Nd:KGW, although most of the work to date had been performed with a frequency-doubled tunable dye laser. The authors discuss a heuristic model developed for evaluating laser options of the REMPI process that considers laser wavelength and pulse energy, duration, and repetition frequency, and describe current studies to determine the overlap of a free-running (i.e., non-tuned) Nd:KGW laser with benzene and toluene absorbance features.

#### Recognition and Quantitation of Closely Related Chlorinated Organic Vapors with Acoustic Wave Chemical Sensor Arrays

Potyrailo, R.A.; R.J. May; T.M. Sivavec.

Internal Standardization and Calibration Architectures for Chemical Sensors.

Proceedings of SPIE - The International Society for Optical Engineering, Vol 3856, p 80-87, 1999

An array of four acoustic wave chemical sensors has been developed and tested for recognition and quantitation of six closely related chlorinated organic vapors at low part-per-million concentrations. The sensor array can detect PCE at as little as 0.2 ppm, TCE at 0.8 ppm, cis-1,2-DCE at 1.4 ppm, trans-1,2-DCE at 1.4 ppm, 1,1-DCE at 3 ppm, and VC in air at 3.5 ppm.

Rejection Basin Detection Using the Integral Spectral Analysis (ISA) Method, Niquelandia, Brazil  
Guimares, Renato Fontes (Univ. de Brasilia (UnB), Brasilia, Brazil); Osmar Abílio de Carvalho Jr.; Ana Paula Martins Ferreira; Mucio Nobre da Costa Ribeiro.

AVIRIS Airborne Geoscience Workshop Proceedings 2001. Jet Propulsion Laboratory, California Inst. of Technology. 4 pp, 2001

In 1973 the Níquel Tocantins Company built a metallurgic complex to produce nickel carbonate from lateritic ore. Nickel carbonate is transported to Sao Paulo, where metallic nickel is produced. The wastes are stockpiled in sedimentation basins around the company. Mainly opaque minerals (maghemite and magnetite) constitute the wastes. The AVIRIS image shows the mill, rejection basins and the dam. This project uses AVIRIS images to characterize the rejection basins formed by opaque minerals.  
[http://popo.jpl.nasa.gov/docs/workshops/01\\_docs/toc.html](http://popo.jpl.nasa.gov/docs/workshops/01_docs/toc.html)

Remote Detection of Methane CH<sub>4</sub> Using a 3.3 $\mu$ m Tunable Lead Salt Diode Laser

Mokhtari, A.E.; N. Cherfi, Laboratoire des Lasers et Applications, Centre de Développement des Technologies Avancées, Algiers, Algeria.

TDLS 98: 2nd International Conference on Tunable Diode Laser Spectroscopy, 6-10 July 1998, Moscow, Russia. Book of Abstracts, p 25, 1998

Lasers constitute a practical and powerful tool to monitor in real time the presence of gaseous pollutants in the atmosphere. The author are studying the detection of methane (CH<sub>4</sub>) using an infrared diode laser and a differential absorption type of detection. The laser system is based on a liquid nitrogen-cooled lead salt diode, with an emission frequency tunable over a 100 cm<sup>-1</sup> bandwidth around 3020 cm<sup>-1</sup> (3.31  $\mu$ m) by adjusting the pumping current intensity and/or the operating temperature. The typical cw emission power is 0.2 mW. CH<sub>4</sub> detection experiments are run in a sample cell containing pure methane at controlled pressures, before extending them to the open atmosphere.

Remote Detection of Nitroaromatic Explosives in Soil Using Distributed Sensor Particles

Simonson, Robert J. (Sandia National Labs.); B.G. Hance; R.L. Schmitt; M.S. Johnson; P.J. Hargis. Detection and Remediation Technologies for Mines and Minelike Targets VI. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4394, p 879-889, 2001

The authors have developed a method that can remotely determine the presence of nitroaromatic explosives in surface soil by utilizing a novel distributed granular sensor approach in combination with UV-visible fluorescence LIDAR (Light Detection and Ranging) technology. Prototype sensor particles have been produced that combine sample preconcentration, explosives sensing, signal amplification, and optical signal output functions. These particles can be sprayed onto soil areas suspected of explosives contamination. By design, the fluorescence emission spectrum of the distributed particles is strongly affected by absorption of nitroaromatic explosives from the surrounding environment. At approximately 1mg/cm<sup>2</sup> coverage of the sensor particles on natural soil, significant spectral changes occur due to TNT concentrations in the ppm range (mg TNT/kg soil) on 2-inch diameter targets at a standoff distance of 0.5 km.

### Remote Electrochemical Sensor for Monitoring Trace Mercury

Wang, J.; B. Tian; J. Lu; D. MacDonald.  
Electroanalysis, Vol 10 No 6, p 399-402, 1998

A newly designed remote probe has been developed for stripping measurements of trace mercury at large sample-instrument distances. Various gold electrodes, stripping modes, and operation conditions have been optimized to render the device suitable for remote monitoring of mercury. The favorable stripping potentiometric response obtained following 0.5-1.0 min deposition leads to a rapid detection of low ppb mercury concentrations, and offers a fast warning capability. The optimized protocol offers a low detection limit and good precision, and the sensitivity, simplicity, stability, and smaller dimensions the new probe have provided good performance for in situ monitoring of trace mercury in natural waters.

### Remote Sensing Using Hyperspectral and Polarization Images

Gupta, Neelam, Army Research Lab.

Instrumentation for Air Pollution and Global Atmospheric Monitoring. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4574, p 184-192, 2002

Relatively compact, lightweight, programmable hyperspectral/polarization imaging systems have been developed based on an acousto-optic tunable filter (AOTF) with different focal plane arrays to cover the spectral range from the visible to the long infrared wavelength region. The spectral region is covered by four separate imagers. An AOTF combined with a tunable retarder can collect polarization signatures as well as spectral signatures, and such spectropolarimetric imagers have been developed for detection in the visible-to-near infrared (VNIR, 0.4-1.0 micrometers) and short wave IR (SWIR, 0.9-1.7 micrometers) regions. A great deal of remote sensing data has been collected using a VNIR spectropolarimetric imager and analyzed using a commercial image processing software program (ENVI). The VNIR imager was used to collect spectral and polarization data from various objects and backgrounds, both in the laboratory and in field tests. This imager uses a tellurium dioxide (TeO<sub>2</sub>) AOTF and a liquid-crystal variable retardation plate with a charge coupled device camera. The spectral images were collected from 0.45 to 1.0 micrometers with a 10 nm step, at two or four polarization settings for each spectral interval. The effectiveness of this system for foliage detection was assessed.

### Renewable Reagent Enzyme Inhibition Sensor for Remote Monitoring of Cyanide

Wang, J. (New Mexico State Univ., Las Cruces); B. Tian; J. Lu; D. MacDonald; J. Wang; D. Luo.  
Electroanalysis, Vol 10 No 15, p 1034-1037, Oct 1998

A renewable-reagent flow probe has been developed for the remote electrochemical biosensing of enzyme inhibitors. The new submersible device addresses the challenges of continuously replacing the inhibited enzyme and consumed substrate. The internal delivery of microliter enzyme and substrate solutions is coupled to an in situ microdialysis sampling of the toxin, and an amperometric detection of the enzymatically generated product. The new concept is demonstrated for the detection of micromolar concentrations of free cyanide in the presence of the enzyme tyrosinase and its catechol substrate. The optimization of various physical and chemical parameters has resulted in a low detection limit of  $2 \times 10^{-6}$  M cyanide and good precision (RSD = 5%). The new device holds great promise for in situ environmental and industrial monitoring of toxins.

### Remote Sensing and Selective Detection of Chemical Vapor Plumes by LWIR Imaging Fabry-Perot Spectrometry

Gittins, C.M. (Physical Sciences Inc.), W.J. Marinelli; J.O. Jensen (U.S. Army Soldier and Biological Chemical Command).

Instrumentation for Air Pollution and Global Atmospheric Monitoring. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4574, p 63-71, 2002

Physical Sciences Inc. has developed and tested two long-wavelength infrared (LWIR) hyperspectral imaging spectroradiometers based on the insertion of a rapidly tunable Fabry-Perot etalon in the field of view of a HgCdTe focal plane array (FPA). The tunable etalon-based optical system enables a wide field-of-view and the acquisition of narrowband (7 to 11  $\text{cm}^{-1}$  spectral resolution), radiometrically calibrated imagery throughout the 8-to-11-micrometers spectral region. The instruments function as chemical imaging sensors by comparing the spectrum of each pixel in the scene with reference spectra of target chemical species.

Results from the Pronghorn Field Test Using Passive Infrared Spectroradiometers--CATSI and AIRIS Jensen, J.O. (U.S. Army Soldier & Biological Chemical Command); J.-M. Theriault (Defence Research Establishment Valcartier, Canada), C. Bradette; C.M. Gittins (Physical Sciences Inc.), W.J. Marinelli. Instrumentation for Air Pollution and Global Atmospheric Monitoring. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4574, p 95-99, 2002

Two passive infrared sensors, the Adaptive InfraRed Imaging Spectroradiometer (AIRIS) and Compact ATmospheric Sounding Interferometer (CATSI), were tested for inclusion into the Joint Service Wide Area Detection Program in the Pronghorn Field Tests held at the Nevada Test Site in 2001. The systems showed good results with various chemicals detected and quantified from a distance of 1.5 kilometers.

A Rugged and Compact Time-of-Flight Mass Spectrometer for Fast and Sensitive Leak Detection Gonin, Marc (Ionwerks, Inc.); K. Fuhrer; M. Ugarov; V. Vaughn; S. Ulrich; M. McCully; A. Schultz. The 3rd Harsh-Environment Mass Spectrometry Workshop, 25-28 March 2002 Pasadena, California.

A compact Time-of-Flight (TOF) mass spectrometer is being developed for air leak detection during the space shuttle start. The main challenges for this application are speed, sensitivity, dynamic range, and ruggedness. The compact TOF prototype contains a rugged, filament-less ionizer, and the advantages and limitations of this ionizer are discussed. The sensitivity of a TOF spectrometer is principally limited by the saturation of the micro-channel-plate detector, which can handle only a few million counts per second, and this paper contains a discussion of an approach to overcome this limitation for this application. A detector scheme is presented that allows users to obtain a dynamic range of  $10^{-6}$  per second with a time-to-digital converter.

<http://cot.marine.usf.edu/hems/workshop/3rdworkshop/program.htm>

Sensing Technologies for Contaminated Sites and Groundwater Dominguez, E. (Univ. of Alcalá de Henares, Madrid, Spain); S. Alcock (Cranfield Univ. at Silsoe, Bedfordshire, UK).

Biosensors and Bioelectronics, Vol 17 No 6-7, p 625 - 633, Jun 2002

This paper is a full summary report on the first SENSPOL Workshop held in Alcalá de Henares, Spain, May 9-11, 2001. A total of 51 papers were presented as lectures and posters addressing the following topics: microtechnology, site investigation and characterization case studies, biomimetic systems, behavior and fate of pollutants, bioavailability and risk assessment, sampling techniques, efficiency control of remediation approaches, multi-parameter sensing, and future directions in development. The conclusions from each session were summarized by an expert chosen to represent each of the topics. In

general, the workshop showed that the development of the field of sensing technologies for environmental monitoring has advanced considerably, particularly with regards to the implementation of fundamental research (e.g., molecularly imprinting polymers, membrane technology, pattern recognition, and transducing schemes), as well as to a more integrated and collaborative approach for the management of European freshwater resources. It is believed that within the next five years some of the technical research will transfer into prototype products for full assessment and evaluation.

#### Short- and Long-Path Laser-Induced Fluorescence in the Water Column for the Detection of Dissolved Chemicals

Sinn, G. (OPTOSENS GmbH), K.-H. Mittenzwey; S. Harsdorf (Carl von Ossietzky Univ. Oldenburg), R. Reuter.

Remote Sensing of Vegetation and Water, and Standardization of Remote Sensing Methods. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3107, p 252-259, 1997

In lidar monitoring of fluorescent and nonfluorescent soluble chemicals in surface water, two signals have to be measured: the total fluorescence lidar intensity  $L$ , which is characterized by long path-lengths of the laser radiation in the water column, and the fluorescence  $F$ , which originates from the first layers immediately below the water surface. The ratio of both intensities  $F/L$  yields the total attenuation coefficient at the laser wavelength for both nonfluorescent and fluorescent substances. A simple experiment in the laboratory with a nitrogen laser was performed on water samples containing algae and a defined amount of humic acid and spiked with fluorescent quinine sulphate and nonfluorescent azobenzene and p-nitrophenol down to ppb concentrations. The attenuation coefficients were measured synchronously by conventional absorption spectroscopy with good correlations between the conventional and the lidar-derived attenuation coefficients. The  $F/L$  ratio seems to be an effective tool for lidar monitoring of dissolved chemicals in water.

#### Simultaneous In-Situ Measurement of $O_2$ , HCl, HF, CO and Dust in Gas from a Waste Incinerator Using Diode Laser Spectroscopy

Bjoroy, O.; I. Linnerud; V. Avetisov; K.H. Haugholt, Norsk Elektro Optikk A/S, Skarer, Norway. The 5th International Symposium on Gas Analysis by Tunable Diode Lasers, Freiburg, Germany, February 1998

Diode laser-based monitors for measuring  $O_2$ , HCl, HF, CO, and dust have been installed in a waste incinerator plant for continuous measurement of emissions and optimization of furnace running conditions. The measurement principle for the gas monitors is wavelength modulation spectroscopy (WMS) using harmonic detection. This paper presents and discusses long- and short-term field measurements. Gas concentrations, in particular the concentration of CO, show large variations on a time scale of less than 15 seconds, which reflects fast changes in the combustion process. The monitors have been running reliably for more than a year, exhibiting performance characteristics that fulfill the requirements for commercial monitors.

[http://www.neo.no/freiburg\\_98.html](http://www.neo.no/freiburg_98.html)

#### Signal Processing Strategies for Passive FT-IR Remote Sensing

Shaffer, Ronald E., Naval Research Lab.

Internal Standardization and Calibration Architectures for Chemical Sensors. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3856, p 12-23, 1999

Computer-generated synthetic single-beam spectra and interferograms were used to study signal processing strategies for two passive Fourier transform IR (FTIR) remote sensing scenarios of four

component mixtures--ethanol, methanol, methyl ethyl ketone, and acetone vapors. Calibration model performance degraded significantly as the uncertainty in plume temperature increased or as the temperature difference decreased, which suggests that in order to quantify passive FTIR spectra remotely, there must be either a large temperature difference or an accurate assessment of plume temperature.

#### Simple Plastic Fiber-Based Optode Array for the In-Situ Measurement of Ground Air Oxygen Concentrations

Koelling, M. (Univ. Bremen), H. Hecht; G.A. Holst (Max-Planck-Institut fuer Marine Mikrobiologie). Advanced Environmental Sensing Technology II. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4576, p 75-86, 2002

A fiberoptical optode array for in situ measurement of oxygen concentrations has been used in both lab and field experiments to monitor subsurface oxygen consumption in lignite mine tailings affected by acid mine drainage formation. The single sensors are constructed from plastic fibers (core diameter 1 mm) with an oxygen-sensitive fluorescent dye film attached to the fiber tip. Measurements were performed with a commercially available oxygen measuring instrument (MICROX 1, PreSens, Regensburg, Germany) modified with the 1-mm plastic fibers. The instrument evaluates the oxygen-dependent change of the luminescence lifetime of an oxygen indicator using a phase modulation technique. The measurement of the pyrite depth distribution of the material confirmed the assumption that the 40-year-old tailings had been depyritized down to a depth of 6 m and that pyrite oxidation and acid mine drainage formation were still going on.

#### A Small Multiple-Pass Time-of-Flight Mass Spectrometer (MR-TOF-MS) for In-Situ Investigations

Casares, A. (II Phys. Inst., Justus-Liebig-Univ., Giessen, Germany); F. Goesmann (Max-Planck Inst. fur Aeronomie (MPIE), Katlenburg-Lindau, Germany), A. Kholomeev, R. Roll, H. Rosenbauer; H. Wollnik (II Phys. Inst., Justus-Liebig-Univ., Giessen, Germany).

Second Workshop on Harsh-Environment Mass Spectrometry, 18-21 March 2001, St. Petersburg, Florida.

To increase the mass resolving power of an energy-isochronous time-of-flight mass spectrometer, the overall flight time of the ions can be increased if the length of the ion pulse is kept constant. The researchers have built a small time-of-flight mass spectrometer in which the ions are repeatedly reflected between two grid-free ion mirrors, thus achieving a mass resolving power that depends on the number of passes of the ions through the system. A multi-pass time-of-flight mass spectrometer (MTOF-MS) was constructed and optimized for in situ investigations in space missions that required a high performance mass spectrometer of very low weight and very small power consumption. In the linear mode (i.e., without reflections), the 420-mm-long system achieves a basic mass resolving power of  $m/Dm=350$  with an electron impact gas ion source operated at a repetition frequency of 1 kHz. In the multi-pass mode the spectrometer achieves a mass resolving power  $m/Dm>4000$  after 15 passes, i.e. after an overall flight path of  $>6.5$  m, which can be increased to a mass resolving power of  $m/Dm>15000$ , after 101 passes, i.e., after an overall flight path of  $>30$  m. The finally registered ion intensity is about 50% of the ion intensity obtained with the MTOF-MS in the linear mode and does not depend on the number of passes. The MTOF-MS will be placed aboard the Lander module of the ROSETTA Mission of the European Space Agency (ESA), which is to be launched in 2003 to perform in situ investigations on the head of the comet P/Wirtanen.

#### Smart 3D Subsurface Contaminant Characterization at the BGRR Decommissioning Project.

Accelerated Site Technology Deployment Cost and Performance Report

Heiser, J. (Brookhaven National Lab., Upton, NY); P. Kalb; T. Sullivan; L. Milian.



Report No: BNL--52666, 84 pp, Dec 2001.

The Brookhaven Graphite Research Reactor (BGR) is currently on an accelerated decommissioning schedule with a completion date projected for 2005. The accelerated schedule combines characterization with removal actions for the various systems and structures. A major project issue involves characterization of the soils beneath contaminated Below Grade Ducts (BGD), the main air ducts connecting the exhaust plenums with the Fan House. The air plenums experienced water intrusion during BGR operations and after shutdown. The water intrusions were attributed to rainwater leaks into degraded parts of the system, and to internal cooling water system leaks. If the characterization could provide enough information to show that soil contamination surrounding the BGD is either below cleanup guidelines or is very localized and can be "surgically removed" at a reasonable cost, the ducts may be decontaminated and left in place, which will provide significant savings compared to breaking up the 170-ft-long concrete duct, shipping the projected 9,000 cubic meters of waste off-site, and disposing of it in an approved facility. The focus of this DOE Accelerated Site Technology Deployment (ASTD) project was to determine the extent (location, type, and level) of soil contamination surrounding the BGD. A suite of innovative characterization tools was used to complete the characterization of the soil surrounding the BGD in a cost-effective and timely fashion and in a manner acceptable to the stakeholders. A state-of-the-art perfluorocarbon tracer (PFT) technology was used to screen the BGD for existing leak pathways and thus focus the characterization on potential contamination hot spots. Once pathways were identified, the sampling and analysis plan was designed to emphasize the leaking areas of the duct and perform only confirmatory checks in areas shown to be leak-free. A small-footprint Geoprobe® was used to obtain core samples and allowed sampling in areas surrounding the BGD that were difficult to access. Two novel, field-deployed, radiological analysis systems (ISOCs and BetaScint™) were used to analyze the core samples and a 3-D visualization system facilitated data analysis/interpretation for the stakeholders. All of the technologies performed as well or better than expected, and the characterization could not have been completed in the same time or at the same cost without using this approach. A total of 904 BGD soil samples were taken, evaluated, and modeled. Results indicated that contamination was primarily located in discrete areas near several expansion joints and underground structures (bustles), but that much of the soil beneath and surrounding the BGD was clean of any radiological contamination. One-year project cost savings are calculated to be \$1,254K. Life cycle cost savings, resulting from reduction in the number of samples and the cost of sample analysis, are estimated to be \$2,162K. When added to potential cost savings associated with decontaminating and leaving the BGD in place (\$7.1 to 8.1M), far greater overall savings may be realized.

[http://www.osti.gov/bridge/product.biblio.jsp?osti\\_id=797955](http://www.osti.gov/bridge/product.biblio.jsp?osti_id=797955)

#### Smart Electronic Nose Using Polymer-Film-Coated Quartz Resonator Gas Sensor for Identification of Harmful Gases

Nanto, Hidehito (Kanazawa Inst. of Technology); Y. Douguchi; K. Yokoi; T. Mukai; J. Fujioka; E. Kusano; A. Kinbara.

Internal Standardization and Calibration Architectures for Chemical Sensors. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3856, p 317-327, 1999

A smart electronic nose containing polymer-film coated quartz resonator gas sensors, based on the solubility parameter of sensing membrane and gases, performs with excellent selectivity and high sensitivity for gaseous forms of toluene, acetaldehyde, and ammonia. The developers found that the solubility parameter is effective to the functional design of the sensing membrane of quartz resonator gas sensors. The identification of each gas kind is made possible by the principal component pattern recognition analysis of the transient response of the each sensor.

## Solid Phase Microextraction as a Sampling Method for Gas Chromatography/Mass Spectrometry in the Field

Hook, Gary (Uniformed Services Univ. of the Health Sciences, Bethesda, MD), Philip Smith; Kenneth Williams (U.S. Army Center for Health Promotion and Preventive Medicine, Edgewood, MD), Michael Sheely.

Second Workshop on Harsh-Environment Mass Spectrometry, 18-21 March 2001, St. Petersburg, Florida.

This paper provides examples of environmental samples collected by solid phase microextraction (SPME) from air (a solvent mixture used in industry), water (the gasoline additive MTBE), and soil (chemical warfare agents). Analyses were performed rapidly through direct exposure of the samples collected on SPME fibers using a field-portable Viking Spectra Trak 572 portable GC/MS system. The SPME sampling was simple for all three types of analytes, involving exposure of the SPME fiber used to the sample headspace (for the solvent and soil samples) or the water that contained the gasoline additive. The SPME method provided a concentrated sample that was easily introducible into the GC injection port for rapid desorption from the SPME fiber by heating. For screening of unknown samples, SPME sampling/sample introduction for GC/MS analysis does not require the typical solvent delay for collection of MS data, allowing examination of early eluting peaks that may be missed when unknown analytes are dissolved in solvent for GC/MS analysis. The SPME sampling method is highly suitable for field use owing to its portability, simplicity of use, broad range of applications, sensitivity, and favorable attributes as a sample introduction method for GC/MS analyses.

<http://cot.marine.usf.edu/hems/workshop/2ndworkshop/presentation.htm>

## Solid-Phase Microextraction (SPME) for Rapid Field Sampling and Analysis by Gas Chromatography-Mass Spectrometry (GC-MS)

Hook, G.L. (Uniformed Services Univ. of Health Science, Bethesda, MD); G.L. Kimm; T. Hall; P.A. Smith.

TrAC - Trends in Analytical Chemistry, Vol 21 No 8, p 534-543, 2002

Solid-phase microextraction (SPME) has been shown to be suitable for sampling environmental contaminants from air, water, and soil for gas chromatography-mass spectrometry (GC-MS) analysis. The paper includes examples of environmental samples collected and analyzed in the field using SPME-GC-MS for qualitative identification of workplace air contaminants from a poorly characterized paint and of gas-phase contaminants present during forensic and clean-up operations following a large fire involving aircraft fuel. In both instances, passive SPME sampling concentrated analytes from the air following short sampling periods and was followed immediately by GC-MS analysis in the field, without further sample preparation. The SPME sampling method is attractive for field use because of its portability, simplicity, broad applications, sensitivity, and favorable attributes as a sample-introduction method for GC-MS analyses.

## Solid Phase Microextraction with Analysis by Gas Chromatography to Determine Short Term Hydrogen Cyanide Concentrations in a Field Setting

Smith, Philip A.; Michael V. Sheely; Timothy A. Kluchinsky Jr.

Journal of Separation Science, Vol 25 No 14, p 917-921, Oct 2002

The authors used 2-minute duration solid phase microextraction (SPME) sampling followed by gas chromatography with a nitrogen-phosphorous detector (GC/NPD) to detect, identify, and quantify airborne hydrogen cyanide (HCN) concentrations in a field setting provided by actuation of two CS riot control canisters in an enclosed building. The presence of HCN was confirmed in the atmosphere sampled by SPME field sampling, followed by gas chromatography with mass spectrometric detection.

With four simultaneous SPME field samples and GC/NPD analysis, the coefficient of variation associated with the HCN peak areas for the samples was 17%, and the HCN concentrations ranged from about 12 to 19 ppm. Acetonitrile and acrylonitrile of undetermined concentration also were detected as volatile nitrogen-containing air contaminants dispersed along with the CS.

#### Spectral Band Characterization for Hyperspectral Monitoring of Water Quality

Vermillion, Stephanie C.; Rolando Raqueno; Rulon Simmons.

AVIRIS Airborne Geoscience Workshop Proceedings 2001. Jet Propulsion Laboratory, California Inst. of Technology. 9 pp, 2001

A method for selecting the set of spectral characteristics (i.e., spectral bandwidth and location) that provides the smallest increase in prediction error is of interest to those using hyperspectral imaging (HSI) to monitor water quality. Three water-quality constituents that can be detected via remote sensing are chlorophyll, total suspended solids, and colored dissolved organic matter. Hyperspectral data provide a rich source of information regarding the content and composition of these materials, but often provide more data than an analyst can manage. Determination of the greatest contribution of these spectral characteristics would greatly improve computational ease and efficiency, and understanding the spectral capabilities of different spectral resolutions and specific regions is an essential part of future system development and characterization. The authors address these issues using data from AVIRIS and a set of models to predict constituent concentrations.

[http://popo.jpl.nasa.gov/docs/workshops/01\\_docs/toc.html](http://popo.jpl.nasa.gov/docs/workshops/01_docs/toc.html)

#### Spectroelectrochemical Sensor for Technetium Applicable to the Vadose Zone

Heineman, William R.; Carl J. Seliskar; Samuel A. Bryan; Timothy L. Hubler, Univ. of Cincinnati, Dept. of Chemistry, Cincinnati, OH.

Report No: DOE-ER62311, 16 pp, Aug 2002

The general aim of this project is to continue the design and implementation of a new sensor technology that offers the unprecedented levels of specificity needed for analysis of the complex chemical mixtures found at DOE sites nationwide. The new sensor concept combines the elements of electrochemistry, spectroscopy, and selective partitioning into a single device that provides three levels of selectivity. The specific goal of this project is the development of a sensor for technetium (Tc) that is applicable to characterizing and monitoring the vadose zone and associated subsurface water at the Hanford site. The first step is to develop a sensor that determines technetium in the chemical form pertechnetate ( $\text{TcO}_4^-$ ). This report summarizes work during June 2001 to June 2002 of a three-year project that began in September 1999. During this period, research efforts have focused on four areas: the electrochemistry of pertechnetate at bare ITO and film-coated ITO electrodes, electrode sensitivity enhancement by increasing analyte absorptivity, development and characterization of selective films, and development of an improved field-portable spectroelectrochemical sensor.

[http://www.osti.gov/bridge/product.biblio.jsp?osti\\_id=798487](http://www.osti.gov/bridge/product.biblio.jsp?osti_id=798487)

#### Spotlight on Diode Lasers

Martin, Phillip, Univ. of Huddersfield, Queensgate, Huddersfield, UK.

Chembytes E-Zine, Jul 1999

Inexpensive, easy to operate, coherent tunable monochromatic light sources from the mid-IR to the UV have been a target of spectroscopists for many years. Apart from conventional absorption and fluorescence spectroscopies, Raman spectroscopy and ellipsometry have benefited from diode lasers as coherent light sources. Diode lasers also have been combined with new high sensitivity techniques such

as intracavity spectroscopy. In fundamental spectroscopy, new laser sources are leading to the structural determination of exotic free radical and cluster species. In atmospheric monitoring, room temperature laser diodes emitting at 8-13 $\mu$ m are a major advance towards improving air quality.  
[http://www.chemsoc.org/chembytes/ezone/1999/martin\\_jul99.htm](http://www.chemsoc.org/chembytes/ezone/1999/martin_jul99.htm)

#### Studies of Perchlorate Triggered Ion-Gate Behavior of sBLM by Electrochemiluminescence and Its Application to a Sensor for Perchlorate

Han, Xiaojun (Changchun Inst. of Applied Chemistry, Chinese Academy of Sciences, Changchun, Jilin, China); Guobao Xu; Shaojun Dong; Erkang Wang.  
Electroanalysis, Vol 14 No 17, p 1185-1190, Sep 2002

The authors found that a supported lipid bilayer membrane (sBLM) made of dimethyldioctadecylammonium bromide (a kind of synthetic lipid), showed ion-gate behavior for the permeation of Ru(bpy)<sub>3</sub><sup>2+</sup> in the presence of perchlorate anion. There existed a threshold concentration (0.1 M) of perchlorate anion for ion-gate opening; below the threshold the ion gate was closed. Above the threshold, the number of opened ion-gate sites increased with the increase of perchlorate anion concentration and leveled off at concentrations higher than 1200 M. Based on these results, a new, reusable sensor for perchlorate was developed.

#### Study of Five Discrete Interval-Type Groundwater Sampling Devices

Parker, Louise V.; Charles H. Clark, U.S. Army Corps of Engineers, CRREL.  
Report No: ERDC/CRREL TR-02-12, 57 pp, Aug 2002

Five relatively recently developed ground-water-sampling devices (the Kabis, HydraSleeve, Discrete Interval, Pneumo-Bailer, and USGS Passive Diffusion Bag [PDB] samplers) were tested to determine their ability to recover representative concentrations of a variety of analytes, including volatile organics, explosives, pesticides, and metals. The first phase of the study included several standpipe experiments with known concentrations of analytes. In the second phase, the devices were used in the field to sample TCE from a deep well and were compared with samples taken using low-flow sampling. The PDB sampler was the easiest device to use but should be used only for selected VOCs. The HydraSleeve and the Kabis Sampler are thief-type samplers that were also relatively easy to use. Although these devices could produce representative concentrations of explosives, pesticides, and metals in the standpipe experiments, they elevated the turbidity in the monitoring well. The authors recommend that their use be limited to wells where the turbidity is not affected by their use, especially if sampling for metals or the more hydrophobic organic contaminants. In addition, there were small but statistically significant losses of some VOCs with the HydraSleeve in the standpipe studies (<5%) and of TCE in the field study (11%). Concentrations of VOCs taken with the Kabis Sampler did not show a substantial and consistent bias in either direction, except for the low-level study where loss of TCE was substantial, 18%. In the field study, loss of TCE was small (<8%) with this device and not statistically significant. The Discrete Interval Sampler and Pneumo-Bailer are pressurized thief-type devices that are designed to collect a sample when activated. The Pneumo-Bailer was heavy and awkward to handle, required taking a nitrogen tank into the field, and was difficult to operate. The Discrete Interval Sampler required only a bicycle pump to pressurize the chamber, was smaller and lighter in weight, and easier to handle and operate than its counterpart. Both devices generally delivered representative concentrations of all the analytes tested in the standpipe experiments. Although loss of TCE was statistically significant for the Discrete Interval Sampler in the field study, loss was very small (<5%).  
<http://www.crrel.usace.army.mil/library/pub02fyo.htm>

Submicron Sensors for Ion Detection Based on Measurement of Luminescence Decay Time  
Koronczy, Ilona (Forschungszentrum Karlsruhe GmbH, Inst. of Instrumental Analysis, Karlsruhe, Germany), Johannes Reichert, Hans-J. Ache; Christian Krause (Inst. of Analytical Chemistry, Univ. of Regensburg, Regensburg, Germany), Tobias Werner, Otto S. Wolfbeis.  
Sensors and Actuators B: Chemical, Vol 74 No 1-3, p 47-53, 2001

Submicron optochemical sensors for pH and chloride were developed by coating silanised optical fibre tips of ~300nm diameter and aluminium-coated SNOM fibres of ~50nm aperture with polymeric membranes containing luminescent indicators. Luminescence decay time was measured using a phase-modulation technique. Changes in decay time are induced by resonance energy transfer from a ruthenium complex (the donor) to the pH indicator bromothymol blue (the acceptor). The donor-acceptor ion pair was immobilized in a hydrogel membrane and underwent a change in decay time with pH. The chloride sensor was made by combining the ion pair for optical transduction with the chloride-carrier tridodecylmethylammonium chloride in a plasticised PVC membrane. Chloride ions present in the solution are carried into the membrane. To maintain electroneutrality, an equivalent molar quantity of protons is coextracted into the membrane where the dye is protonated.

Supersonic Jet Spectroscopy for Environmental Analysis  
Imasaka, Totaro, Kyushu Univ.

Environmental Monitoring and Remediation Technologies. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3534, p 573-581, 1999

Supersonic jet spectrometry combined with multiphoton ionization mass spectrometry has been developed to detect dioxins, halogenated benzenes, and phenols at ultratrace levels. Laser pulses at either 150-fs or 500-fs were used as an excitation/ionization source and the results compared with those obtained using a 15-ns laser pulse. The ionization yield was substantially improved by decreasing the laser pulsewidth. A collinear ionization scheme resulted in sensitivity enhancement by a factor of 50. Supersonic jet spectrometry was tested for the detection of halogenated aromatic hydrocarbons formed by thermal decomposition of polyvinyl chloride and chlorinated polyvinyl chloride.

Technology Transfer Project Final Report—"Fast" Gas Chromatography/Mass Spectrometry  
Dioxin/Furan Analysis Method  
MSE Technology Applications, Inc., Butte, MT.  
Report No: PTP-75, 64 pp, Sep 2000

The objective of the Accelerated Polychlorinated Dibenzo-p-dioxins/Dibenzofurans Sampling and Analysis (APSA) project, previously known at the "Fast" Gas Chromatography/Mass Spectrometry (GC/MS) Analysis project, is to develop, test, and demonstrate an APSA system capable of on-site sampling and analyses of dioxins/furans in incineration offgases with a turnaround time of 2 hours. The APSA device is intended to be used for diagnostic rather than compliance monitoring; however, an advanced version may be suitable as a substitute for U.S. EPA Method 23. Normal turnaround time for Method 23 and other standard methods of dioxin/furan sampling and analysis is 1 month or more. To better understand factors affecting dioxin/furan formation and to control and minimize emissions, it would be helpful to have a faster dioxin/furan sampling and analysis method. Accordingly, under the direction of DOE, MSE Technology Applications, Inc., originated and is now testing an accelerated sampling and analysis system based on analytical thermal desorption techniques. This sampling and analysis system is expected to have a turnaround time of as little as 2 hours, or potentially less than 2 hours where higher detection limits resulting from abbreviated sampling times (less than 1 hour) are permissible.

<http://tmfa.inel.gov/Documents/technical.asp>

Test Plan for the Demonstration of Geophysical Techniques for Single-Shell Tank Leak Detection at the Hanford Mock Tank Site, Fiscal Year 2001

Barnett, D.B.; G.W. Gee; M.D. Sweeney, Pacific Northwest National Laboratory, Richland, WA.  
Report No: PNNL-13598, 97 pp, Jul 2001

This report describes tests conducted by CH2M HILL Hanford Group, Inc. at Mock Tank 105-A to assess the applicability of geophysical methods (electrical resistance tomography, high resolution resistivity, cross-borehole seismography, cross-borehole radar, and cross-borehole electro-magnetic induction) to the detection and measurement of single-shell tank leaks into the vadose zone during planned saltcake dissolution operations. Of primary importance in the testing is the determination of minimum time for a method to detect a leak, the method's capability to quantify leak volumes, the capability of the method to detect staged leaks (superimposed leaks), and an estimated cost of an operational system in a tank farm. Deployment of multiple methods will also provide an opportunity for comparison of results from independent data sets. In parallel with the geophysical tests, a Partitioning Interwell Tracer Test study will be conducted simultaneously at the Mock Tank to assess the effectiveness of the technology in detecting and quantifying tank leaks in the vadose zone. Preparatory and background work using cone penetrometer methods will be conducted at the Mock Tank site and an adjacent test area to derive soil properties for groundtruthing purposes for all methods.  
<http://vadose.pnl.gov/files/contrepts/pnnl-13598.pdf>

Testing of a Continuous Sampling Mercury CEM at the EPA-Rotary Kiln Incinerator Simulator Facility

Baldwin, D.P.; S.J. Bajic; D.E. Eckels; D.S. Zamzow, Ames Laboratory, Ames, IA.  
Report No: IS-5151, 25 pp, Apr 2002

This report has been prepared to document the performance of the continuous sampling mercury monitoring system developed by Ames Laboratory for use as a continuous emission monitor (CEM) and funded by DOE. The purpose of the project is to develop instrumentation and methods for spectroscopic field-monitoring applications. During FY01 this included continued development and testing of an echelle spectrometer system for the detection of mercury (Hg) by atomic absorption. Due to the relatively poor limits of detection for Hg by optical emission techniques, the CEM has been designed for the detection of elemental Hg by optical absorption. The sampling system allows continuous introduction of stack gas into the CEM for analysis of elemental and total Hg in the gas stream. A heated pyrolysis tube is used in this system to convert oxidized Hg compounds to elemental Hg prior to analysis for total Hg. The pyrolysis tube is bypassed to measure elemental Hg. The CEM is designed to measure the elemental Hg concentration of the gas sample, measure the total Hg concentration, perform a zero check (analysis of room air), and then re-zero the system to correct for any instrumental drift that occurs over time. This is done in an automated, sequential measurement cycle to provide continuous monitoring of Hg concentrations in the stack gas. The continuous sampling Hg CEM was tested at the EPA-Rotary Kiln in Durham, NC, at the beginning of FY02. This report describes the characteristics and performance of the system and the results of the field tests performed at EPA.  
[http://www.osti.gov/bridge/product.biblio.jsp?osti\\_id=797632](http://www.osti.gov/bridge/product.biblio.jsp?osti_id=797632)

Thermal Oxidative Pyrolysis and Evolved Gas Analysis (TOPEGA): An In Situ Test Bed for Compositional Analyses of Soil, Rock, or Ice Samples

Dissly, Richard; William Horsley, Ball Aerospace & Technologies.  
In Situ Instruments Workshop, 11-13 June 2002, Pasadena, California. NASA, Jet Propulsion Laboratory, Center for In-Situ Exploration and Sample Return.

Thermal oxidative pyrolysis and evolved gas analysis (TOPEGA), a current PIDDP study at Ball Aerospace & Technologies Corp., is a flexible breadboard test system consisting of a miniature, reusable thermal analyzer (TA) and evolved gas analysis (EGA) detectors. This test bed is intended to assess both individual component and system-level performance for potential use in analytical in situ instrumentation for future planetary surface missions. TA designs that have been tested include both a differential scanning calorimeter and differential thermal analyzer, each run on multiple mineral and ice samples. Gaseous pyrolysis products are analyzed by the EGA, consisting of a suite of different solid-state, compound-specific detectors (for the detection of H<sub>2</sub>O, CO<sub>2</sub>, SO<sub>2</sub>, O<sub>2</sub>, H<sub>2</sub>, and NO<sub>x</sub>) and an FTIR analyzer.

#### Tiny Time-of-Flight (TOF) Mass Spectrometer for Biodetection

Bryden, Wayne A., Johns Hopkins Univ. Applied Physics Laboratory, Laurel, MD.  
Second Workshop on Harsh-Environment Mass Spectrometry, 18-21 March 2001, St. Petersburg, Florida.

The matrix-assisted laser desorption/ionization (MALDI) technique has revolutionized biological mass spectrometry. Using this technique, large molecules (particularly proteins) can be employed as signature biological materials. These signatures have been used with the proper algorithms to identify microorganisms down to the strain level using mass spectrometry. With DARPA funding, the system is being developed to carry this technology into the field in a package with a low logistics burden and only light training needed for operators. The system has demonstrated rapid classification and identification of a variety of bioaerosol components including bacteria (both spores and vegetative cells), viruses, and toxins. The biodetection system includes an optimized mass analyzer with tandem capabilities, an automatic collection system for transport of concentrated airborne particle samples into the mass analyzer, an automated analytical methodology, and automated signal processing, decision aids, and data displays. This system is applicable to the rapid (<5minute) identification of airborne microorganisms in a mixed environment.

<http://cot.marine.usf.edu/hems/workshop/2ndworkshop/presentation.htm>

Toolkit for the Rapid Screening and Characterization of Waste Piles on Abandoned Mine Lands  
Smith, Kathleen S. (U.S. Geological Survey); D.L. Campbell; G.A. Desborough; P.L. Hageman; R.W. Leinz; M.R. Stanton; S.J. Sutley; G.A. Swayze; D.B. Yager.

Progress on Geoenvironmental Models for Selected Mineral Deposit Types. U.S. Geological Survey Open-File Report 02-195, Chapter C, p 55-64, 2002

There are thousands of historical mine-waste piles present on inactive metal-mining sites, some of which are on Federal lands and have been abandoned. Assessment of metal mobility, acid-drainage production, and toxic effects from the weathering of historical mine-waste piles is an area of growing need as the environmental effects of inactive mine-waste sites across the country are being evaluated and mitigated. The U.S. Geological Survey Mine Waste Characterization Project has taken a multidisciplinary approach to assemble, develop, and refine methods and tools for characterizing and screening weathered solid-mine wastes. Researchers from a variety of disciplines, including geophysics, geochemistry, analytical chemistry, geology, mineralogy, remote sensing, and spatial modeling, have worked together at metal-mining waste sites in Colorado and New Mexico to develop an integrated "toolkit" for the rapid screening and characterization of historical mine-waste piles. Tools developed from this work can be used in ranking and prioritizing historical mine-waste piles. This chapter contains a brief discussion of some tools for sampling and geochemical screening, non-invasive screening (e.g., imaging spectroscopy and geophysical methods), and site characterization (e.g., mineralogy determination by x-ray diffraction, metal partitioning determination by sequential chemical extractions, isolation and enumeration of iron- and sulfur-oxidizing bacteria).

<http://pubs.usgs.gov/of/2002/of02-195/>

#### Trace Analysis of Lead at a Nafion-Modified Electrode Using Square-Wave Anodic Stripping Voltammetry

Crowley, Karl; John Cassidy, Dublin Inst. of Technology, Dublin, Ireland.  
Electroanalysis, Vol 14 No 17, p 1077-1082, Sep 2002

Anodic stripping voltammetry (ASV) using square-wave voltammetry was applied with Nafion-coated glassy carbon electrodes for lead analysis. At square-wave frequencies greater than 100 Hz, the system could be employed satisfactorily for trace lead detection down to 1 ppb.

#### Transparent Oxygen Optodes in Environmental Applications at Fine Scale as Measured by Luminescence Lifetime Imaging

Holst, Gerhard A. (Max-Planck-Institut fuer Marine Mikrobiologie); U. Franke; B. Grunwald.  
Advanced Environmental Sensing Technology II. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4576, p 138-148, 2002

The MODular Luminescence Lifetime Imaging system (MOLLI) makes it possible to use oxygen sensors that are not optically isolated: transparent planar optodes and dispersed nano-optodes enable a direct optical link between the chemical parameter to be measured (e.g., oxygen) and the structure that is responsible for the distribution of the chemical parameter (e.g., ascidian and corals). The spatial resolution of the MOLLI imaging system is determined by the area size of the view field that is imaged onto the amount of pixels of the CCD-chip (640x480) and by the spatial limitations of the sensing layer. The paper contains examples of biological marine applications.

#### Tunable Diode Lasers: Tunable Diode Lasers Are Increasing Their Market Penetration via Rapid Evolution: a New Generation of Products Every Year or So

Shine, Bob; Tim Day, New Focus, Inc., Santa Clara, CA.  
Lasers & Optronics, p 13-14, March 1998

The tunable diode laser (TDL) has become a successful product with applications ranging from telecommunications to spectroscopy to metrology. While each of these applications places slightly different requirements on the laser and the user interface, each of them requires a narrow-linewidth, continuously tunable, reliable source. TDL technical capabilities and features play a major role in the success of the product, as well as its ease of use. With TDL technology, researchers can imagine a very sensitive diode-laser-based sensor for combustion monitoring. While the pace of development in the tunable laser field has been quite fast, with a new laser system available almost every year, each new generation has offered customers additional benefits. Additional wave-lengths such as the 2-micrometer TDL and products tailored to customer needs have allowed customers to do what they could not have done before and provided simpler, easier-to-use tools for them. This focus on customer needs continues to expand the market for an already successful technology.

#### Ultra-High-Sensitivity Passive FTIR Sensor (HiSPEC) and Initial Field Results

Schildkraut, E.R. (Block Engineering), R.F. Connors; A. Ben-David (Science and Technology Corp.); A.I. Ifarraguerri (U.S. Army Edgewood Chemical Biological Ctr.).  
Instrumentation for Air Pollution and Global Atmospheric Monitoring. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4574, p 18-25, 2002



The HiSPEC instrument was designed to examine the potential for passive detection of sub-lethal concentrations of toxic materials and to test the potential for passive indication of a biological agent in air. Some subtle differences between the laboratory and field performance of HiSPEC since 1999 have been diagnosed with the aid of HiSPEC's precise internal sampling system, the results of which may have implications for improving less sensitive passive field systems.

#### Underwater Mass Spectrometers for Detection of VOCs and Dissolved Gases

Kibelka, Gottfried (Center for Ocean Technology, Univ. of South Florida); Tim Short; David Fries.  
The 3rd Harsh-Environment Mass Spectrometry Workshop, 25-28 March 2002 Pasadena, California.

The researchers have developed and deployed mass spectrometry systems capable of autonomous underwater operation for chemical analysis for the purpose of analyzing coastal marine waters for natural and anthropogenic organic compounds and gases. The high spatial and temporal resolutions of the underwater mass spectrometer (MS) systems has been used to monitor and map chemical distributions in harsh environments. The underwater mass spectrometers are housed in separate pressure vessels that are connected in series for deployment. The front vessel serves as the sampling system and contains a peristaltic pump and a 4-port valve. Sample water and charcoal cleaned sample water are alternately pumped into the hollow fiber membrane in the central vessel by switching the valve. The central pressure vessel contains the MS itself, a membrane probe, the turbo molecular/drag pump and a Card PC. The back vessel contains two dry diaphragm pumps in series that serve as backing pumps for the turbo molecular/drag pump. This approach allows the evacuation of the diaphragm-pump pressure vessel at the beginning of each operation, which extends the endurance of continuous operation to longer than a week. Battery powered deployment duration is currently limited to two hours for the ion trap and four hours for the quadrupole MS. All parts can be activated and controlled via Ethernet from an external computer. For gaseous compounds and very volatile organic compounds, an Inficon Transpector quadrupole residual gas analyzer is used. The analyzer has been tested on dissolved gasses in shallow marine thermal vents and VOCs in wastewater influent, water plant and rivers. For trace compounds and pollutants, a Varian Saturn 2000 ion trap analyzer is used to attain higher sensitivity and the optional advantages of MS/MS systems. The underwater ion trap system has been used to detect plumes of VOCs in Tampa Bay water.

<http://cot.marine.usf.edu/hems/workshop/3rdworkshop/program.htm>

#### Use of Stable Isotopes to Monitor the Natural Attenuation of Dicyclopentadiene

Stehemier, L.G. (Nova Chemicals Ltd., Calgary, AB), L. Cooke, R. Hornett; R. Aravena (Waterloo Univ., ON).

Proceedings of the 25th Arctic and Marine Oilspill Program (AMOP) Technical Seminar, 11-13 Jun 2002, Calgary, AB (Canada). Environment Canada, Environmental Technology Centre, Ottawa, Ont. Vol 2, p 907-920, 2002 [NTIS: DE20259944]

Stable isotope fractionation is a method used to prove that residual hydrocarbons from an oil spill are being naturally attenuated in soil and ground water. Hydrogen isotopes and carbon isotopes are the two isotopes that have been used to provide this evidence. Evaporation, adsorption and biodegradation are among the processes that can cause fractionation of isotopes. However, the largest fractionations take place during biodegradation because of the unidirectional characteristics of metabolism and the thermodynamic selectivity of enzymatic processes in biological systems. This paper presents the results of a monitored natural attenuation program for hydrocarbons in soil and ground water at a chemical plant in Alberta where dicyclopentadiene (DCPD) was biodegraded. DCPD is a co-product from the cracking of ethane to ethylene. Piezometers were used to monitor the stable isotope fractionation of DCPD over a three year period. Evidence that DCPD was biodegrading was the fact that the change in carbon-13 was enriched 4.1% in one study area during the monitoring period. The results are among the

first definitive proof that DCPD biodegrades in the field. Analysis by gas chromatography-carbon-isotope ratio mass spectrometry is an essential technique for monitoring recalcitrant, low water-soluble hydrocarbons.

Use of Vertical-Radar Profiling to Estimate Porosity at Two New England Sites and Comparison with Neutron Log Porosity

Buursink, M.L. (CGISS, Boise State Univ., Boise, ID); J.W. Lane Jr., (OGW-BG, U.S. Geological Survey, Storrs, CT); W.P. Clement (CGISS, Boise State Univ.), M.D. Knoll.

Proceedings: Symposium on the Application of Geophysics to Engineering and Environmental Problems, Las Vegas, Nevada, February 10-14, 2002. Environmental and Engineering Geophysical Society, Denver, CO. CD-ROM, 12 p.

Vertical-radar profiles (VRPs) and neutron porosity logs were acquired at two sites in New England: Haddam Meadows State Park in Connecticut and Massachusetts Military Reservation on Cape Cod. Both sites include boreholes drilled to depths from 30 to 50 meters into unconsolidated fluvial or glacial sediments. The VRP data are inverted using Tikhonov regularization to obtain interval radar propagation velocities. The interval radar propagation velocities from the VRPs are converted to estimates of saturated sediment porosity using the Topp and time-propagation petrophysical models. VRP-derived porosities are compared to neutron log-derived porosities and yielded a correlation between values derived from the two methods. Overall correlation between the VRP-derived porosities and the neutron log-derived porosities supports the advantage of deriving porosities from VRP data due to the decreased cost and ease of data acquisition, and simple processing and inversion routines. [http://water.usgs.gov/ogw/bgas/publications/SAGEEP02\\_12GW5/](http://water.usgs.gov/ogw/bgas/publications/SAGEEP02_12GW5/)

User's Guide for Polyethylene-Based Passive Diffusion Bag Samplers to Obtain Volatile Organic Compound Concentrations in Wells, Part 1: Deployment, Recovery, Data Interpretation and Quality Control and Assurance

Vroblecky, Don A., U.S. Geological Survey, Columbia, SC.

USGS Water-Resources Investigations Report 01-4060, 25 pp, 2001

Water-filled passive diffusion bag (PDB) samplers described in this report are suitable for obtaining a variety of VOCs in ground water at monitoring wells. The suggested application for PDB samplers is for long-term monitoring of VOCs in ground-water wells at well-characterized sites. Where the screened interval is greater than 10 ft, the potential for contaminant stratification and/or intra-borehole flow within the screened interval is greater than in screened intervals shorter than 10 ft. It is suggested that the vertical distribution of contaminants be determined in wells having 10-ft-long well screens, and that both the vertical distribution of contaminants and the potential for intra-borehole flow be determined in wells having screens longer than 10 ft. A typical PDB sampler consists of a 1- to 2-ft-long low-density polyethylene lay-flat tube closed at both ends and containing deionized water. The sampler is positioned at the target horizon by attachment to a weighted line or fixed pipe. The amount of time that the samplers should be left in the well prior to recovery depends on the time required by the PDB sampler to equilibrate with ambient water and the time required for environmental disturbances caused by sampler deployment to return to ambient conditions. The rate that water within the PDB sampler equilibrates with ambient water depends on multiple factors, including the type of compound being sampled and the water temperature.

<http://sc.water.usgs.gov/publications/difsamplers.html>

User's Guide for Polyethylene-Based Passive Diffusion Bag Samplers to Obtain Volatile Organic Compound Concentrations in Wells, Part 2: Field Tests

Vroblecky, Don A. (ed.), U.S. Geological Survey, Columbia, SC.

USGS Water-Resources Investigations Report 01-4061, 102 pp, 2001

This report presents six case studies where passive diffusion bag (PDB) samplers were tested under field conditions. The sites represent two U.S. Naval facilities (Naval Air Station North Island, CA, and Naval Industrial Reserve Ordnance Plant Fridley, MN), and three U.S. Air Force facilities (Davis Global Communications, CA, Hanscom AFB, MA, and McClellan AFB, CA). The primary ground-water contaminants of interest were chlorinated hydrocarbons. Most of the case studies are previously published reports or their summaries.

<http://sc.water.usgs.gov/publications/difsamplers.html>

Using an optical sensor to quantify the amount of oil, water, and gas in a water-continuous flow

Wu, Xu; E.B. Dussan; O.C. Mullins, Schlumberger-Doll Research.

Internal Standardization and Calibration Architectures for Chemical Sensors. Proceedings of SPIE - The International Society for Optical Engineering, Vol 3856, p 298-307, 1999

An optical probe system has been developed to monitor the volume fractions and flow rates of crude oil, water, and gas at each point of entry along the well. It uses a laser- or LED- beam directed to the tip of a tiny optical probe situated in the flow stream. By measuring the reflection from the probe tip, gases can be distinguished from liquids by the large difference in refractive index. Fluorescence characteristics of crude oils can distinguish oil from non-oil. By integrating the time fraction of individual events in reflection and fluorescence respectively, the volume fraction of the three phases can be determined. The leading edge of the fluorescence signal indicates the speed of the oil drops, which, combined with the volume fraction of oil, gives the oil flow rate. The system requires no calibration for the volume fraction measurement; however, a simple calibration is needed for determining the oil drop speed. This describes the response of different probe designs.

Using AVIRIS Data to Map Geologic Signatures of Copper Flat Porphyry Copper Deposit, Hillsboro, New Mexico

Penn, Brian S. (Boeing-Autometric, Inc., Colorado Springs, CO); Eric Livo (U.S. Geological Service Lakewood, CO).

AVIRIS Airborne Geoscience Workshop Proceedings 2001. Jet Propulsion Laboratory, California Inst. of Technology. 10 pp, 2001

The most popular software package for processing hyperspectral imagery is the Environment for Visualizing Imagery (ENVI) available from Research Systems, Inc. Other available lesser-known software packages include the system developed at the USGS Spectroscopy Laboratory, called Tetracorder (previously known as Tricorder). Tetracorder is an in-house tool used almost exclusively by the members of the USGS Spectroscopy Laboratory. Tetracorder has been used successfully at the Summitville mine in southwestern Colorado, the Leadville superfund site, and Yellowstone Park. Another relatively unknown product with unique classification capabilities is the Kohonen self-organizing map(s) (SOM). Each of these products was applied to the AVIRIS imagery of Copper Flat porphyry copper deposit (CFPCD) in south-central New Mexico. SOM proved to be a useful addition to the hyperspectral toolkit.

[http://popo.jpl.nasa.gov/docs/workshops/01\\_docs/toc.html](http://popo.jpl.nasa.gov/docs/workshops/01_docs/toc.html)

Using Time Domain Reflectometry for Non-Aqueous Phase Liquid Saturation Measurements

Persson, Magnus, Dept. of Water Resources Engineering, Lund Univ., Sweden.

TDR 2001: Innovations in Applications of Time Domain Reflectometry. Proceedings, 5-7 September 2001, Northwestern University, Evanston, Illinois. p 362-373, 2001

Detailed laboratory experiments were conducted to investigate the relationship between time domain reflectometry (TDR) measurements and the concentration of nonaqueous phase liquids (NAPL) in soils. Calibration was made in homogeneous sand using three different NAPLs. It was shown that the previously used mixing model led to errors up to 0.05 m<sup>3</sup> m<sup>-3</sup> for saturated soils. In unsaturated soil, it was shown that measurements of only  $K_a$  can not be used for estimation of  $q_{NAPL}$  even if  $q_w$  is known; instead, the TDRs capability of determining both  $K_a$  and bulk electrical conductivity ( $s_a$ ) was utilized to estimate  $q_w$  and  $q_{NAPL}$ . The approach presented in this study can be used for simultaneous observation of  $q_w$  and  $q_{NAPL}$  during NAPL transport experiments in both unsaturated and saturated soils. <http://www.iti.northwestern.edu/tdr/tdr2001/proceedings/>

#### UV-VIS Spectroscopy of 2,4,6-Trinitrotoluene-Hydroxide Reaction

Felt, D. R. (Applied Research Assoc., Inc., Southern Div., Vicksburg, MS); S.L. Larson (U.S. Army Engineer Research and Development Center, Vicksburg, MS); E.J. Valente (Mississippi College).  
Report No: ERDC/EL TR-02-22, 75 pp, Aug 2002

Base-induced transformation (BIT) of explosives has shown promise as a rapid, low-cost technology for remediating explosives in soil and water. When used as a restoration technology, the BIT process incorporates the addition of highly basic material to the soil or groundwater, resulting in the transformation of the parent compound. Ideally, the process would drive the degradation of the parent to environmentally benign compounds. Although the BIT process has been known for decades, the majority of work reported has been related to treating much higher concentrations than are generally found on sites requiring remediation. The mechanism and products of the Hydroxide- (OH-) 2,4,6-Trinitrotoluene (TNT) reaction at concentrations of environmental concern are poorly understood. Previous kinetics studies of the OH-TNT reaction have only considered the reduction of the TNT analyte concentration, not the reaction of intermediates or final products. During these previous studies, TNT quickly degraded in less than 40 minutes at room temperature in basic solution, but the overall OH-TNT reaction may not have been completed. Though the final products of the OH-TNT reaction may be benign, intermediate products may be toxic to inherent bacteria or bind with environmental matrices. Identification and quantification of the reaction mechanism and all reaction components (reactants, intermediates, and final products) of the OH-TNT reaction are necessary to determine the technical feasibility of BIT as a remediation technology. The rate constants for each step in the reaction derived from the reaction mechanism could be used to guide engineers and technicians responsible for designing and operating the technology. Detailed study of the mechanism of degradation and the interactions of the individual degradation products requires an analytical technique that enables separation of the individual compounds. Typically, the individual reaction components are separated using techniques such as liquid chromatography and identified using mass spectroscopy. Unfortunately, the final products of the OH-TNT reaction make this process problematic because of limitations on standard separation techniques. The polymers that form as a result of the OH-TNT reaction often foul the separation column because of their large molecular size. To overcome this difficulty, the study reported here evaluates an alternate technique, ultraviolet-visible (UV/VIS) spectral analysis, to obtain similar information using factor analysis of kinetic spectral data. The knowledge of basic properties of the OH-TNT reaction presented in this report adds to the understanding of the BIT process.  
<http://www.wes.army.mil/el/elpubs/genrep.html>

#### Variation in Aluminum, Iron, and Particle Concentrations in Oxidic Groundwater Samples Collected by Use Of Tangential-Flow Ultrafiltration with Low-Flow Sampling

Szabo, Z. (U.S. Geological Survey), J.H. Oden, J. Gibs, D.E. Rice; Y. Ding (New Jersey Inst. of Technology).

Chemical and Biological Early Warning Monitoring for Water, Food, and Ground. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4575, p 42-61, 2002

Particulates that move with ground water and those that are artificially mobilized during well purging could be incorporated into water samples during collection and could cause trace-element concentrations to vary in unfiltered samples, and possibly in filtered samples (typically 0.45-um (micron) pore size) as well, depending on the particle-size fractions present. Therefore, measured concentrations may not be representative of those in the aquifer. Ground water may contain particles of various sizes and shapes that are broadly classified as colloids, which do not settle from water, and particulates, which do. This paper describes an investigation of variations in trace-element concentrations in ground-water samples as a function of particle concentrations and particle-size fractions.

VOC Emission Source Strengths of Tankers During Refuelling Activities Determined by Spectroscopic Remote Sensing and Inverse Dispersion Modeling

Schaefer, K. (Fraunhofer-Institut fuer Atmosphaerische Umweltforschung); H. Hoffmann; I. Dormuth; C. Jahn; S.M. Emeis.

Remote Sensing of Clouds and the Atmosphere VI. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4539, p 247-257, 2002

The VOC emissions of tankers were investigated in a river harbor with fence-line monitoring by differential optical absorption spectroscopy (DOAS). Benzene, toluene and p-xylene concentrations were measured by a mono-static DOAS using 3 retro-reflectors, and an inverse method was applied on the basis of these non-intrusive measurements of effluent concentrations in the exhaust plume and meteorological measurements to determine the emission source strengths. Emissions resulted from the unloading and loading of gasoline, from ventilation of storage tanks of tankers into ambient air, and from using the land-site gasoline vapor recovery unit in a tank farm for ventilation.

Volcanic Monitoring Using Field-Portable Mass Spectrometers: Towards On-Site and Real-Time Gas Analysis at Fumaroles

Diaz, Jorge A., Univ. de Costa Rica, San Jose, Costa Rica.

Second Workshop on Harsh-Environment Mass Spectrometry, 18-21 March 2001, St. Petersburg, Florida.

In situ mass spectrometer measurements of volcanic gaseous emissions were conducted at fumarolic sites in volcanoes of Hawaii, Costa Rica, and California. For validation, gas concentrations obtained by MS agreed with values obtained using GC at the Hawaiian Volcano Observatory for both in situ and traditional bottle sampling. Several other tests have been conducted in volcanoes in Costa Rica and California to demonstrate the power of field-portable mass spectrometry for real-time continuous volcanic gas monitoring of species such as He, CO<sub>2</sub>, SO<sub>2</sub>, and H<sub>2</sub>S. A commercial quadrupole mass spectrometer (QMS-300 from Stanford Research Systems) and a newly developed Field-Portable Compact Double-Focusing Mass Spectrometer were deployed in the measurement program. The ultimate goal of the project is to establish a network of low cost miniature mass spectrometers located near the rim of each volcano to monitor on-site and in real time the key gases released by the volcano and connected to internet through wireless communication to each local observatory. The measuring instruments would be accessible through the web from any point of the planet to provide data shared by diverse interested parties.

<http://cot.marine.usf.edu/hems/workshop/2ndworkshop/presentation.htm>

Water Monitoring of Polycyclic Aromatic Hydrocarbons by Laser-Excited Time-Resolved Shpol'skii Spectrometry with Fiber Optic Probes

Campiglia, Andres D.; Adam Bystol, North Dakota State Univ.

Advanced Environmental Sensing Technology II. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4576, p 196-206, 2002

A method has been developed for routine monitoring of polycyclic aromatic hydrocarbons in water samples. Method innovations include a rapid solid-liquid extraction procedure, a cryogenic fiber-optic probe for fluorescence measurements in frozen matrices at liquid helium temperature (4.2 degrees K), and an instrumental system for laser-excited time-resolved Shpol'skii spectrometry. The authors illustrate the potential of the monitoring method with the results from the direct trace analysis of 15 EPA priority pollutants in less than five minutes.

Wireless Remote-Query Environmental Monitoring Using Magnetoelastic Sensors

Ong, Keat Ghee (Pennsylvania State Univ.); C.A. Grimes; M.K. Jain; C. Mungle.

Advanced Environmental Sensing Technology II. Proceedings of SPIE - The International Society for Optical Engineering, Vol 4576, p 169-180, 2002

Magnetoelastic sensors made of amorphous metallic glass ribbons or wires have been used to measure environmental parameters such as temperature, humidity, viscosity, and chemical concentration, including pH, carbon dioxide, and ammonia. This paper describes the operating principles of the magnetoelastic sensors and presents several proven applications, as well as methods for optimizing the sensor performance. A remote detection of the shift in the resonant frequency of the magnetoelastic sensors determines the parameter of interest, which is dependent upon factors that include stress, pressure, temperature, and magnetic field.

## **EPA SBIR Awards**

EPA Contract Number: 68D02009

Areté Associates, P.O. Box 6024, Sherman Oaks, CA 91413

Cindy S. Orser, PI, (818) 501-2880

Apr 1, 2002 - Sep 1, 2002

\$70,000

The Application of MASC Technology to the Problem of Contaminant Monitoring for the Water and Wastewater Industries (EPA 2002 SBIR Phase I)

Modeling of active site chemistry (MASC) is a technology being developed by Arete Associates to address problems concerning the inherent fragility associated with biological materials. MASC technology seeks to reduce complex biological systems down to their essential components and then simulate them with stable synthetic entities. The benefits of this approach are increased stability of the sensor element, reduction in cost to produce and manufacture the device, and the ability to miniaturize components. As a proof-of-principle for the application of MASC technology to water monitoring, Arete Associates has constructed an amperometric nitrate sensor by modeling the enzyme nitrate reductase. Under amperometric conditions, the modified electrode exhibits a linear sensitivity to nitrate at levels starting at 3 ppm NO<sub>3</sub>-N, up to 100 ppm NO<sub>3</sub>-N. The Phase I proposal will provide funding to complete the feasibility study of the amperometric sensor through continued characterization of the electrode selectivity, extended testing of electrode stability (robustness), nitrate analysis with standard EPA drinking and wastewater solutions, and sample analysis provided by third-party water and wastewater professionals. A field-testable prototype sensor to be used as a portable device or as an in-line monitor will be built. The Phase I prototype will serve as a platform technology that will be advanced to a multicontaminant analytical device during the Phase II funding period through the addition of newly developed specific chemical detection electrodes for water contaminants of interest, including nitrite, cyanide, phosphate, chromium, mercury, and MTBE.

EPA Contract Number: 68D02020  
Eltron Research, Inc., 4600 Nautilus Court, South, Boulder, CO 80301-3241  
Michael T. Carter, PI, (303) 530-0263  
Apr 1, 2002 - Sep 1, 2002  
\$69,995  
Fiber Optic DNAPL Monitor (EPA 2002 SBIR Phase 1)

Eltron Research, Inc., will develop a fiber-optic sensor that uses a solvatochromic probe to reversibly detect the presence and nature of contaminants. The Phase I project will address the development of sensor materials and chemistry, neural network-assisted data interpretation, and design of a sensor system that can identify and quantify contaminants. Fiber optic sensors capable of ppb-level detection of hydrocarbons, including fuels and chlorinated hydrocarbons, will find immediate commercial application in monitoring leakage from storage facilities and detection of immediate contamination and health hazards in work areas where these materials are used or stored.

EPA Contract Number: 68D02022  
Fayette Environmental Services, Inc., P.O. Box 30, Fayette, MO 65248  
Rhys N. Thomas, PI, (660) 248-1911  
Apr 1, 2002 - Sep 1, 2002  
\$70,000  
Real-Time Analysis of Metals in Aqueous Waste Streams (EPA 2002 SBIR Phase 1)

The proposed innovation, a new form of spectrometry, will be able to quantify the metals in aqueous effluents to 100 ppb in real time. Some industries accumulate aqueous wastes until analysis has been completed; others discharge the wastes and hope that the analysis will be favorable. The first method incurs significant storage costs, the latter incurs significant liability. The proposed instrument, cost-comparable to existing analytical techniques, obviates the need for accumulation and removes most of the potential liability. A real-time monitoring system can prevent many inadvertent discharges of toxic metals if the monitoring system controls the outlet valve. The proposed analytical method, pioneered 50 years ago, could not be applied to real-time analysis until fast and inexpensive computers with large memories and storage devices became available. The computational requirements for resolving complex spectra are significant, but well within the range of personal computers and existing mathematical packages. Because the technique is new, the proposed system requires that thousands of new constants be generated. The immediate objective of this research is to measure the necessary constants and demonstrate that the mathematical theory can be applied to a real problem. Phase I will result in an instrument that lacks only the user interface software, which will be developed by Fayette Environmental Sciences, Inc., in Phase II for the prototype instrument. Phase II will include a demonstration of the prototype in parallel with an existing analytical system. Being cost comparable to existing analytical methods, the instrument will be attractive to industries that generate metal-laden wastewater. In addition to meeting the analytical burden cost effectively, the instrument will reduce liability by documenting all discharges in small increments of time. The instrument also will find application in monitoring process baths for trace metals contamination. The same instrument may be modified to analyze metals in gaseous effluent with detection limits below current regulatory levels.

EPA Contract Number: 68D02025

Frontier Geosciences, Inc., 414 Pontius Avenue, North, Seattle, WA 98109

Hakan Gurleyuk, PI, (206) 622-6960

Apr 1, 2002 - Sep 1, 2002

\$70,000

A Portable Spectrometer for the Accurate Determination of Arsenic in Waters (EPA 2002 SBIR Phase 1)

Frontier Geosciences, Inc., proposes to develop a portable field analyzer for the determination of low levels of arsenic in waters. The instrument will employ the principle of hydride generation-microplasma-atomic fluorescence spectrometry, and it is anticipated that the instrument will be able to analyze approximately 20 samples per hour, with detection limits of approximately 0.1 µg/L. The method will use a novel type of hydride-generation vessel, in which the hydride-generation reaction can be conducted in a closed atmosphere, thereby protecting the operator from arsine exposure. The arsines formed in the vessel will be swept into the microplasma atomization cell, where they decompose and then are detected by atomic fluorescence spectroscopy. The field analyzer will be operated using portable power generators and controlled by a laptop computer. Portable devices of this kind are specifically requested by EPA in their Small Business Innovation Research Request for Proposals for the year 2002, to eliminate the need to pack and ship samples to distant laboratories as well as to obtain real-time information at lower costs. In Phase I, Frontier Geosciences, Inc. proposes to build and optimize a prototype atomic fluorescence detector and the novel closed hydride-generation vessel. The two then will be coupled to determine the analytical performance characteristics of this technology, and the suitability of this instrument for field analysis will be demonstrated. In Phase II, a market-ready instrument will be designed that (after modifications) also may be suitable for arsenic speciation and for the field determination of other inorganic priority pollutants, such as mercury or selenium.

EPA Contract Number: 68D02034

OPOTEK, Inc., 2233 Faraday Avenue, Suite E, Carlsbad, CA 92008

Eli Margalith, PI, (760) 929-0770

Apr 1, 2002 - Sep 1, 2002

\$69,995

A New Compact Portable Field Instrument for Continuous Real-Time Measurement of Trace Organic Air Pollution Emissions Using Jet-REMPI Mass Spectrometry (EPA 2002 SBIR Phase 1)

The goal of this project is to couple a compact tunable ultraviolet laser system with a jet-resonance-enhanced multiphoton ionization (REMPI) time-of-flight mass spectrometer to provide a fieldable system for real-time concentration measurements of aromatic hazardous air pollutants (HAPs) in urban air environments. The jet-REMPI technique already has proven to be powerful for the measurement of HAPs at low detection limits (ppt) with high chemical specificity. However, this technique currently requires a complex and delicate laser source, which confines the instrument to the laboratory. By developing a truly portable device, measurements can be taken in the field with both high temporal and spatial resolution, data that are essential components of emissions modeling, dispersion modeling, source apportionment, and ultimately, human exposure modeling. This information cannot reliably be estimated or inferred by any current method, but must be acquired through actual field measurements under typical, time-varying ambient human exposure conditions. Despite the need for such data, reliable ambient concentrations have been measured for fewer than 40 percent of the 189 HAPs, which lends urgency to the development of a field jet-REMPI instrument to help fill gaps in the data. Phase I research will involve the design of a compact optical parametric oscillator laser specifically tailored for the jet-REMPI application and testing of the laser on the current mass spectrometer system at SRI International. Measurements with calibrated simulated air samples will be made for both neat compounds and mixtures of HAPs. The detection limits and chemical specificity



performance of the system will be compared with the results already obtained at SRI. With performance validation, a design for a complete integrated jet-REMPI system for Phase II field tests will be generated.

#### 1 EPA 2003 Phase I

EPA Contract Number: 68D02090

Thomas E. Coleman, PI, (509) 454-5094

dTEC Systems, LLC, 3012 16th Avenue West, Seattle, WA 98119

Oct 1, 2002 - Jul 31, 2003

\$100,000

Real-Time Multi-Parameter Analysis of Pollutants in Stormwater and Other Complex Analyte Matrices Using Electrospray Ionization-Ion Mobility Spectroscopy (EPA 2003 SBIR Phase 1)

The objectives of dTEC Systems during this Phase I research project include determining the practical detection limits, range, response time, and reproducibility of measurement for chemical species representative of the most common urban stormwater pollutants using ESI-IMS. Additional objectives will be to evaluate the potential for interferences that might limit the applicability of the method for some analytes, and to assess the effectiveness of sample filtration and other inline sample pretreatment steps in maximizing the amount of chemical information that can be obtained using ESI-IMS. Completion of the Phase I objectives will make possible, during Phase II, the development and field testing of a working prototype ESI-IMS instrument for real-time monitoring of stormwater discharges and combined sewer overflows (CSOs). The ability to continuously monitor a wide range of inorganic and organic pollutants throughout the duration of a storm event would greatly improve the characterization of pollutant loads as well as the effectiveness of best management practices for stormwater treatment. With nearly 4,000 communities in the United States required to obtain permits for stormwater discharges, and 772 of these communities having CSOs with a total of 9,471 CSO discharges, the potential market for a cost-effective multianalyte instrument as proposed in this research is significant. Additional commercial opportunities that could be readily implemented include the monitoring of drinking water for arsenic and disinfection by-products and the monitoring of wastewater for conventional and priority pollutants.

#### EPA 2002 Phase 2

EPA Contract Number: 68D02053

Miniaturized Electrochemical Sensor for Cr(VI) in Groundwater and Surface Water (EPA 2002 SBIR Phase 2)

Veronica M. Cepak, PI,

Eltron Research Inc., 4600 Nautilus Court, South Boulder, CO 80301-3241

Jun 1, 2002 - Jun 1, 2004

\$224,995

This project will utilize photolithography and microfabrication in the assembly of a Cr(VI) monitoring device that is compact, portable, and cost effective. The proposed sensor will be a self-contained laboratory that samples, analyzes, and stores the results of onsite testing under a variety of sampling conditions. The device will rely on the pressure-driven introduction of aqueous samples that will be combined with a small, specific volume of electrolyte. Analyte streams of arbitrary ionic strength and composition will be sampled with minimal pretreatment. The use of a microelectrode array sensor chip

will allow for increased sensitivity via enhanced diffusion of the analyte to the sensor element. In addition, use of a miniaturized detector will reduce solution waste during testing. Eltron Research, Inc.'s proposed electrochemical detection scheme allows for the use of simple, inexpensive instrumentation that is capable of the remote monitoring of groundwater and surface waters for Cr contamination. Phase II will focus on the optimization of the proposed Cr(VI) sensor in addition to the assembly and design of a prototype unit for field analysis of groundwater and surface waters using minimal analyte and supporting electrolyte. In Phase I, Eltron successfully demonstrated that self-assembled monolayer (SAM) modified microelectrode arrays could be used for the electrochemical detection of Cr(VI) in aqueous solutions. Cr(VI) solutions with concentrations varying from 0.1 ppb to 100 ppb could be detected using a sensitive electrochemical method. Using photolithography, a robust microelectrode array was fabricated and incorporated into a microfluidic flow cell for Cr(VI) detection. Furthermore, this flow cell was successfully coupled to a peristaltic pump to introduce analyte and supporting electrolyte for Cr(VI) detection, and was interfaced to benchtop electrochemical instrumentation (a potentiostat) for potential use in long-term monitoring situations. The performance of the miniaturized Cr(VI) detector was studied as a function of such variables as pH, supporting electrolyte concentration, SAM deposition time, Cr(VI) exposure time, electrolyte type, and Cr(VI) concentration. The electrochemical detection of Cr(VI) in water is a cost-effective method for long-term, remote monitoring of suspected environmental contamination sites. This approach could find general use in both specific EPA applications and those of the private sector; for example, the monitoring of Cr waste in the electroplating industry. Other industries requiring wastewater monitoring for hexavalent chromium include metal processing, galvanic plants, tanneries, wood preservation, chemical manufacturing, aerospace, and electronics.

[http://cfpub.epa.gov/ncer\\_abstracts/index.cfm/fuseaction/search.welcome](http://cfpub.epa.gov/ncer_abstracts/index.cfm/fuseaction/search.welcome)

EPA Contract Number: 68D02058

AGCS Sensor for Gas Leak Detection (EPA 2002 SBIR Phase 2)

Nelson, Loren D., PI, (303) 933-2200

OPHIR Corporation, 10184 W. Belleview Ave., Suite 200, Littleton, CO 80127

Jun 1, 2002 - Jun 1, 2004

\$224,999

OPHIR Corporation's (OPHIR) Phase I project was very successful. All tasks identified in the Phase I proposal were met and exceeded. The results of Phase I modeling and trade studies indicate that OPHIR's proposed technology exceeds expectations for sensitivity and detection range. Field test data have demonstrated that OPHIR's technology—a sensor that uses a new Active Gas Correlation Spectrometer (AGCS)—can achieve a sensitivity of 50 ppb for methane, and 33 ppb for ethane. This technology holds great promise for meeting the needs of several applications within the natural gas industry. This project is focused on developing a cost-effective remote sensing system to detect methane and ethane (the two primary constituents of natural gas). Ethane is an excellent indicator of natural gas because it is scarce within the natural environment and not associated with other common combustible gases. Consequently, this system will provide a significant cost savings to the natural gas industry by reducing the time and effort required to find natural gas leaks and eliminating efforts to investigate false alarms. This technology will provide the essential detector currently needed to reduce the atmospheric emission of methane, a significant greenhouse gas. The Phase II effort provides the next logical step toward developing this technology for introduction into the marketplace. During Phase II, OPHIR will perform several test programs with the prototype hardware. This includes supporting the U.S. Department of Energy's (DOE) CO<sub>2</sub> Sequestration Project, performing airborne flight testing, performing a leak detection survey with a local gas utility company, and completing an extensive field test for a private corporation. OPHIR already has received significant financial commitments from private industry and DOE's National Energy Technology Laboratory to support this Phase II effort.

These commitments exceed \$140,000. OPHIR has gained the support of Xcel Energy, which will be providing engineering and test evaluation support.

EPA Contract Number: 68D02051

A New Biosensor for Rapid Identification of Bacterial Pathogens (EPA 2002 SBIR Phase 2)

Mary Beth Tabacco, PI, (703) 658-7692

Echo Technologies Inc., 5250 Cherokee Ave., Alexandria, VA 22312

Jun 1, 2002 - Jun 1, 2004

\$224,965

Rapid, handheld or portable instrumentation for determining the quality of natural waters, recreational waters, and distributed and treated supplies does not currently exist. Echo Technologies, Inc., completed a Phase I project that demonstrated a new approach for the identification of bacteria in aqueous systems. The approach uses bacteriophage as the molecular recognition element. Bacteriophage are virus particles that generally attach to and infect a narrow range of host cells. Biosensors based on this molecular recognition offer a rapid, selective, and potentially very sensitive method to detect bacteria and bacterial pathogens in potable and recreational waters. Feasibility of the concept was demonstrated by fabricating fluorescently labeled virus probes (FLVPs) to detect and identify bacteria for representative waterborne bacteria, including: *Escherichia coli*, *Enterococcus faecalis*, and *Vibrio natriegens* bacteria. The preparation of FLVPs has been made quite reproducible. The adhesion to host cells is very rapid, good selectivity was demonstrated in samples with host cells and mixtures, and the response from a solid-phase FLVP biosensor was demonstrated. Several experiments were conducted with a customized detection system to demonstrate the feasibility of making a small in-line instrument capable of high-sensitivity detection. These cumulative results lay an excellent foundation for the Phase II development effort. In Phase II, a prototype rapid bacteria identification system will be designed, fabricated, and evaluated in the laboratory and at an independent test facility. The heart of the instrument will be an array of encoded FLVPs integrated with a charge coupled device (CCD)-based imaging/detection system. Application of the FLVP technology to solid-state optical sensing represents a new approach to real-time detection of bacterial pathogens. This approach will minimize the need for culturing to identify pathogens, and is an important departure from immunoassay- or DNA-based sensing concepts. The miniature probes are perfectly suited for incorporation in a sensor array for the simultaneous detection of many bacterial pathogens.

EPA Contract Number: 68D02046

Remote Sensing Instrument for Particulates and NOx From Heavy-Duty Diesel Vehicles (EPA 2002 SBIR Phase 2)

J. Barry McManus, PI, (978) 663-9500

Aerodyne Research Inc., 45 Manning Rd., Billerica, MA 01821

Jun 1, 2002 - Jun 1, 2004

Project Amount: \$224,647

Aerodyne Research, Inc., is developing a remote sensing device for particulate emissions by extending its gaseous pollutant laser instrument designs. This novel approach probes the exhaust plume with several coaligned laser beams that have a range of wavelengths from mid-infrared to visible. All of the beams sample the same absorption path, simultaneously measuring the column density of soot and gaseous pollutants. Multiple wavelength opacity is used to determine the mass density of soot. Multiple wavelengths yield a more precise measurement of opacity, and hence, more accurate soot density. Multiple wavelength measurement also has the potential to distinguish changes in particle characteristics with varying engine state. During Phase I, both theoretical and experimental

investigations were conducted to determine the practicality of multiwavelength opacity measurements for the remote sensing of diesel soot. A prototype instrument that remotely measures opacity at three wavelengths simultaneously with CO<sub>2</sub> at a data rate of 25 Hz was assembled and tested. This instrument has been tested in the laboratory and outside the laboratory, including measurements of plumes of passing automobiles and a diesel fuel pool fire. The results were highly successful and encouraging. The instrument demonstrated sufficient sensitivity to measure soot densities at current fleet average emissions from heavy-duty diesel vehicles. Simultaneously, CO<sub>2</sub> was measured with a noise level of 25 ppm-m. In Phase II, Aerodyne Research, Inc., will build new instrumentation that employs the multiple wavelength particulate system. This instrumentation will be extended to include more wavelengths, and possibly will include scatter information for particle sizing. Quantum cascade lasers will be used for the mid-infrared spectroscopic measurement of gaseous pollutants, allowing for a noncryogenic system. The integration of these techniques into one instrument will provide a powerful tool for survey measurements of both PM and NO<sub>x</sub> emissions of heavy-duty diesel engines in real-world situations, with the mix of engine loads encountered in normal driving. Phase II efforts will be conducted in association with a commercial partner that builds remote sensing instruments to detect motor vehicle pollution.