FOREWORD

This special journal issue contains select papers from the *2006 International Symposium on Spectral Sensing Research (2006 ISSSR)* that fall into the subject matter areas of: (1) Multispectral/Hyperspectral Techniques for Water Monitoring Applications; and (2) Frontier Spectroscopic Science and Technology for Chemical, Biological and Radiological (CB&R) Defense. The specific focus of the *2006 ISSSR* was on the creation of new technology-program oriented networks that will serve as a research and development foundation for the advancement of the state-of-the-art in spectroscopic-based early-warning sensor capabilities. In recent years, spectral sensing has experienced rapid technical advancement that has led to practical field sensors. Therefore spectral-based techniques exhibit the clear potential for providing more effective, economical and supportable (i.e., reagentless) solutions to military and homeland defense early-warning monitoring requirements for water, surface and air related sensing applications.

An increased emphasis on *reagentless* spectroscopy is motivated primarily by performance issues associated with traditional chemical and biological (CB) point and standoff techniques. In particular, sensors have been previously developed and fielded that rely heavily on reagents and/or burdensome support structures that are expensive and difficult to maintain and that have serious false alarm issues. Previously implemented technologies include biological assays, mass spectrometry and ion mobility. Other explored methodologies include novel materials (mips, smart ligands, amino acid sequences, aptamers, sol gel, aerogel, electro-conducting polymers, etc.) or bulk property interactions (electrochemistry, surface acoustic wave, surface plasmon resonance, thermal capacity) and combinations of the two.

At this time, extensive expertise exists in the multispectral/hyperspectral community for applications such as airborne and space-based sensing and imaging which has proved effective in monitoring weather, resource management (agriculture, forestry), oil/mineral deposits and CB detection in air releases. Hence, spectral-based techniques clearly have potential for providing near to mid-term solutions for many of the monitoring problems associated with CB&R contaminations of water, surfaces and air. However, the ultimate realization of such spectroscopic techniques will probably require the fusion of many types of spectral-sensing techniques and modality. Therefore, standoff and point interrogation sensors are now sought that can provide for extremely high confidence in CB&R detection and monitoring scenarios and the goal of the *2006 ISSSR* and this

companion special issue is to organize and focus the science and technology base towards these important challenges.

This special issue begins with a collection of research and development papers on the subject of spectroscopic techniques for "Water Sensing and Monitoring." These papers address the Joint Services issued formal requirements for new capabilities in early warning monitoring of water supplies against a CB event. These requirements put a new type of problem on the table that is considered to be "non-traditional" in a number of ways. Specifically, new ways of thinking and innovative approaches and technology are needed to solve this problem. For example, the civilian and military drinking water providers have extensive history, expertise and a proven track record that is unsurpassed at delivering high quality, safe drinking waters to their customers. But these standards and monitoring methods were developed to address traditional public health requirements, to be able to protect the public health in a court of law and to provide a level of validated data that could be used to guide or modify treatment protocols over extended time periods. Detection is based on classical laboratory methods that require extensive sample collection, handling, transportation, labor, and logistics. Hence, it is accepted and expected to take days to conduct and weeks to report.

In contrast the Joint requirements call for "early warning" monitoring. "Early warning" must be "real-time", "in-line", low cost, low labor, easy to support, maintain and use. A mandate for "reagent less" technologies is given to reduce costs of disposables, logistics support, contamination and fouling in the field. An early warning monitor is not developed as a tool for "detect-to-treat" or "detect-to-sue", but simply as a type of smoke-alarm to "detect-to-warn" to alert a population of an abnormal toxic or pathological event. It must provide enough time so that people can reduce or eliminate catastrophic exposure. The goal is to prevent human morbidity and mortality. It may also be used as a trigger to invoke more extensive and classical methods for forensic confirmation or treatment.

The Standoff Detection and Spectral Sensing communities are accustomed to rapid data acquisition and reporting, early warning monitoring and contamination avoidance. Standoff Detection was created and developed for the purpose of early warning and contamination avoidance. They have worked since the 1960s to develop the types of technologies that can provide this type of monitoring for air and more recently surfaces, but historically have not been asked to address water. Water for these communities is considered a "non-traditional" background and has not received consideration or dialogue. A deep well of technological capability exists in this community and it needs to be pumped for water answers. To this end, the goal of the ISSSR 2006 water monitoring session was to bring together these different expert communities to foster new thoughts and collaborations, identify new approaches, new ways of using existing

technologies, highlight emerging and enabling technologies with the focus on developing new and novel solutions to answer the Joint Service Requirements.

This special contains a very good representative sampling of the papers that were presented at the *2006 ISSSR* on the subject of spectroscopic techniques for "Water Sensing and Monitoring." In particular, the special issue begins with papers that focus on the subject of real-time, on-line monitoring of drinking water distribution networks for both chemical and biological agent threats. The subject matter then shifts towards innovations such as chip-size wavelength detectors that allow for highly accurate and spectrally broad, compact spectrometers for optical identification of bio-agents in fluids, and multi-color native fluorescence spectroscopy that enables identification of multiple classes of bio-molecules. This special issue also contains papers from the diverse subject areas: Water quality monitoring using satellite imagery; Deep UV laser-induced fluorescence (LIF) for the detection of trace species and dissolved organic compounds in water; and, Materials and sampling protocols for effective coupling to miniaturized and portable FTIR for aqueous-based detection of toxic compounds. Papers are also included that focus on emerging techniques such as: Terahertz spectroscopy of proteins in water that utilize both direct absorption and circular dichroism; and, a novel Surface enhanced Raman Spectroscopy (SERS) active material with enhanced sensitivity, specificity and speed in detecting chemical agents and their hydrolysis products. The water monitoring section concludes with the two novel sample preparation methodologies: Front-end liquid flow cells which utilize electric field concentration methods for collecting spores onto the surface of an attenuated total reflection (ATR) IR crystal; and, Liquid-Flow concentration with a reversible filter that enables preconcentration of microorganisms into a tiny volume of liquid for enhanced spectral detection.

This special issue also contains a collection of technical papers on the subject of "Frontier and Emerging Spectroscopic Science and Technology" that have relevance to a general array of CB&R defense and security applications. Here, the initial focus of this issue is on new scientific techniques and advanced technology that offer the potential for enhancing and extending the effectiveness of existing hyperspectral/multispectral sensing methodologies. Examples of these research and development efforts include: Adaptive spectrometers and multispectral imagers that allow for real-time optimization of standoff CB sensor data; Physics-based algorithms for the more effective detection of gaseous effluents using airborne LWIR hyperspectral imagery of complex scences; Application of combined infrared and Raman spectroscopy for collecting the vibrational signatures of chemical warfare agent simulants, their hydrolysis and degradation products and a number of toxic industrial compounds (TICs); Development of double-transducer noncollinear acousto-optic tunable filter (AOTF) cells that enable enhanced visible to midwave infrared spectral imaging; Demonstration of a remotely operable miniature spectrometer for the detection of TICs using near infrared spectroscopy; Utilization of multidimensional phase shaped femtosecond pulses to control the fragmentation and

ionization of mass spectrometry; New insights into surface-plasmon-resonance phenomenon for optical sensing applications; Demonstration of an optical characterization unit based upon fluorescence spectroscopy-on-a-chip that utilizes a compact fluidic platform to achieve point detection and analysis of pathogens; and, Enhanced UV light emitting diodes with higher efficiencies, increased power and extended lifetimes for reagentless bio-agent detection and water purification.

The later portion of this special issue is on novel technology and phenomenology that has potential for impacting spectroscopic-based sensing in the future. Some examples of these research and development efforts include: Identification of a novel semiconductor-based hetero-systems that allows for the design of an optically-triggered interband resonant-tunneling-diode (OT-I-RTD) oscillator capable of producing significant levels of terahertz (THz) frequency output power; Presentation of a novel THz detector concept that is based upon magnetoresistance oscillations in two-dimensional electron systems in semiconductors that allows for the simultaneous determination of the radiation frequency and intensity from a simple electrical measurement; Investigations of a novel quantum-mechanical phenomenon associated with the electromagnetic response of cold-atom systems that offers the potential for completely new sensing modalities from RF to the far-infrared (terahertz); Studies on dilute-magnetic-semiconductor (DMS) based multi-barrier structures offering a new type of very high speed transistors for integrated sensor applications at THz frequencies; Research on InN and Inn/InGaN nanostructures that show their promise for THz sources pumped by low cost 1550 nm fs fiber and CW lasers; Introduction of a novel type of fluctuation-enhanced sensing that exploits the information contained in microfluctuations to increase both selectivity and sensitivity of conventional chemical sensors; Quantification of phenomenology of time-resolved visible, near- and mid-IR spectra from fast-transient high-explosive fireballs showing its utility for explosive classification; Development of a new broadband Chirped-Pulse Fourier Transform Microwave (CP-FTMW) spectrometer that allows for high resolution and high throughput analysis of chemical warfare agents even when present in mixtures; Studies that quantify the environmental effects on the THz spectra of DNA and on the THz spectra of nanostructures useful for the study of the vibrational, electronic and optical properties of DNA; Demonstration of a compact ultrasensitive wideband superconducting mm/submm integrated digital spectrometer for chemical and biological agent detection; Illustration of the effectiveness of laser-ionization mass spectroscopy for the detection of explosives and chemical warfare agents; Development of in-line optical fiber structures that allow for large interaction lengths and high sensitivity in surface plasmon and evanescent sensors for chemical and biological agents; Design of functional surfaces for application in point sensing of a single or a few bio-molecular targets to enable label-free ultra-low concentration detection; Development of hybrid films that possess fluorescence intensity dependency on exposure to methanol vapors; and, Introduction of a novel nanoscale imaging technology for application in THz-frequency transmission microscopy based sensing.

Finally, the organizing committee *2006 ISSSR* and the Editors of this special issue would like to recognize the following Best Paper Presentations that lead off this collection of technical papers:

Programmable Adaptive Spectral Imagers for Mission-Specific Application in Chemical/Biological Sensing
By Neil Goldstein, *Spectral Sciences, Inc*

Design & Optimization of an I-RTD Hybrid THz Oscillator Based Upon $In_{1-x}Ga_xAs$ /$GaSb_yAs_{1-y}$ Heterostructure Systems
By Weidong Zhang, *North Carolina State University*

Study of Transport and Devices Based on the Photo-Excited Two-Dimensional Electronic System
By Ramesh Mani, *Harvard University*

Editors:
Janet Jensen, U.S. Army Edgewood Chemical Biological Center
Dwight Woolard, U.S. Army Research Office