Communication Products

FOR THE

Environmental Management Science Program

FY2001 Year-End Summary

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COVER GRAPHIC: Dr. Paul P. Woskov, Massachusetts Institute of Technology, along with his co-principal investigators Dr. T. Bond Calloway Jr, Savannah River Technology Center, and Dr. S. Kamakshi Sundaram, Pacific Nothwest National Laboratory, has received a R&D 100 Award for his work on the Millimeter-Wave Measurements of High Level and Low Activity Glass Melts. The device uses coherent millimeter waves to measure the viscosity of high temperature melts. The viscosity is a very important property in the creation of high-level and low-activity glass waste forms. Precise control of the viscosity is necessary to provide the proper pouring parameters, proper mixing of the contaminants and the glass matrix and extending melter refractory lifetime. This device has a greater viscosity measurement range than its competitors, is more accurate, and can withstand higher temperatures. It will also have applications outside the EM Program [see Project #81897, renewal of #65435].

EXECUTIVE SUMMARY

The Environmental Management Science Program (EMSP) was established by Congress in 1996 under the Department of Energy (DOE) Environmental Management (EM) Office of Science and Technology to "develop and fund a targeted long-term basic research program that will result in transformational or breakthrough approaches for solving the Department's environmental problems." The EMSP is a partnership between the Department of Energy (DOE) Office of Basic and Applied Research and the Office of Science, and funds competitively awarded research that seeks scientific understanding leading to reduced remediation risks, costs, or schedules, and helping to solve currently intractable problems. As such, EMSP supports research that leads directly to the fulfillment of the following EMSP research objectives:

- Provide scientific knowledge that will revolutionize technologies and clean-up approaches to significantly reduce future costs, schedules, and risks

- "Bridge the gap" between broad fundamental research that has wide-ranging applicability such as that performed in DOE's Office of Science and needs-driven applied technology development that is conducted in EM's Office of Science and Technology

- Focus the nation's science infrastructure on critical DOE environmental management problems.

The intent of this *EMSP Communication Products Summary* is to provide information concerning varied research transition activities. Research transitions are measures of how successfully the program has transitioned knowledge gained from research projects to other areas. These measures may be in the form of actual transfers of new knowledge or data gained through research products or processes to other areas within EM, such as Focus Areas and Crosscutting Programs, or may be more general knowledge transfer measures found in similar research programs, such as collaborations, numbers of student researchers, peer reviewed papers and presentations (communication products), or consultations.

Since 1996, the EMSP has funded over 300 basic research projects at 90 universities, 13 national laboratories, and 22 other governmental and private laboratories in 39 states and 7 countries. Many of these projects have generated sufficient technical data and identified specific, potential field applications to warrant movement into the applied R&D arena. Communications products from EMSP-funded projects, with total quantities in each category as follows:

Type of Publication/Presentation	*Total*
Journal Articles	674
Media Reports	1
Other (Encyclopedias, manuscripts)	45
Papers	38
Patent disclosures and applications	37

Posters	60
Presentations	833
Press Releases	6
Proceeding Contributions	185
Reports	68
Theses/Dissertations	52

The information presented in this volume is an attempt to capture research publications and other communications products as of October 31, 2001, and, therefore, should not be considered to be a complete or accurate listing. Research transition activities for EMSP-funded projects are documented in *Research Accomplishments for the Environmental Management Science Program*.

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Introduction

RESEARCH ACCOMPLISHMENTS FOR THE ENVIRONMENTAL MANAGEMENT SCIENCE PROGRAM

INTRODUCTION

The Environmental Management Science Program (EMSP) is a partnership between the Department of Energy (DOE) Office of Basic and Applied Research and the Office of Science. The mission of the EMSP is to develop and fund a targeted long-term basic research program that will result in transformational or breakthrough approaches for solving the Department's environmental problems. The EMSP funds competitively awarded research that seeks scientific understanding leading to reduced remediation risks, costs, or schedules, and helping to solve currently intractable problems. The sites will use the understanding gained through EMSP-supported research to improve their cleanup efforts. Implementing these approaches will lead to reductions in cleanup costs, as well as reductions in risks to workers and the public. The Environmental Management Science Program (EMSP) has funded over 300 basic research projects at 90 universities, 13 national laboratories, and 22 other governmental and private laboratories in 39 states and 7 countries.

Many EMSP projects have generated sufficient technical data and identified specific, potential field applications to warrant movement into the applied R&D arena. Based on the technical strength of his work for Project #81897 (renewal of #64535), *Millimeter-Wave Measurements of High Level and Low Activity Glass Melts*, Dr. Paul P. Woskov, Massachusetts Instutite of Technology, has received an R&D 100 Award for the creation of a new device that uses coherent millimeter waves to measure the viscosity of high temperature melts. Viscosity is an important property in the creation of high-level and low activity glass waste forms. This device has a greater viscosity measurement range than its competitors, is more accurate, and can withstand higher temperatures. It has a broad range of applications in non-EM Programs as well (see cover photo).

The information contained in this document has been gathered from various sources, such as interactions with EMSP staff, proceedings from EMSP workshops and technical conferences, principal investigators, the Project Tracking System, EMSP Project Annual Reports, and literature searches. The information presented is an attempt to capture research transition activities and therefore should not be considered to be a complete or accurate listing. This document contains the best available data as of October 31, 2001.

Problem Areas Addressed by EMSP Research

The EMSP focuses on the key EM problem areas defined in the *EM Research and Development Program Plan*. These problem areas are grouped by waste area, representing the scope of cleanup facing EM. These areas are the basis for developing science and technology investments. The focus areas link both research and technology development to these eight problem areas:

- *Deactivation and Decommissioning* research advances science to solve environmental problems associated with placing equipment and structures in a desired end state. Desired end states include complete removal and remediation of the facility, release of the facility for unrestricted use, or release of the facility for restricted use.

- *High-Level Waste* research advances science to solve environmental problems associated with storage tanks containing highly radioactive wastes, which include organic and inorganic chemical compounds in solid, colloidal, slurry, and liquid phases.

- *Mixed Low-Level Waste (MLLW) /Transuranic Waste (TRU)* research advances science to solve environmental problems associated with very limited treatment options and disposal capacities.

- *Nuclear Materials* research advances science to solve environmental problems associated with unstable materials, such as plutonium metals and oxides, highly enriched uranium and nuclides of other actinide elements, and the long-term storage of stabilized materials.

- *Spent Nuclear Fuel* research advances science to solve environmental problems associated with safely and efficiently managing spent nuclear fuel from both domestic and foreign reactors.

- *Subsurface Contamination* research can assist the Department in solving environmental problems associated with hazardous and radioactive contaminants in soil and groundwater that exist throughout the DOE complex, including radionuclides, heavy metals, and dense, nonaqueous phase liquids.

- *Health, Ecology, and Risk* is a crosscutting problem area; therefore, the research investment will impact cleanup work across the Department of Energy (DOE) complex. There is scientific uncertainty about the levels of risk to human health and the environment at the end stages of the DOE cleanup effort. Accurate risk analyses require thorough knowledge of contaminant characteristics, basic ecological processes and principles, rates at which contaminants move through ecosystems, and health and ecological effects. In particular, better knowledge of radionuclide and toxic chemical transport dynamics and the potential effects of long-term exposure to low levels of radionuclides, in combination with other contaminants, is needed to assist the DOE in its efforts to protect the public, workers, and the environment. This research would also improve the understanding of threatened and damaged ecosystems and processes to restore their viability and quality.

- *Long-Term Stewardship* research supports issues that impact the Department in assessing site conditions after a site is closed and a remedy has been implemented. Long-term stewardship research is necessary to support the Department's commitment to protect human health and the environment after site closure for sites where cleanup to levels acceptable for unrestricted use is not possible.

Science Categories

EMSP research is classified further within each problem area based upon the type of science being conducted. Science classifications include the following:

- Actinide Chemistry including uranium, americium, and plutonium
- Analytical Chemistry and Instrumentation includes sensor development and diagnostics such as non-destructive examination
- Biogeochemistry studies such as oxidation/reduction and biological degradation
- Engineering Science research such as robotics and remote sensing
- Geochemistry that focuses on reactions within the subsurface
- Geophysics that included advanced characterization methods
- Health Science research on dose assessment, bio-markers, and risk estimates
- Hydrogeology that targets subsurface transport mechanisms and predictive modeling
- Inorganic Chemistry including tank waste speciation and metals remediation
- Low Dose Radiation to understand the health effects of low doses of radiation
- Materials Science which studies phenomena such as corrosion, glasses and other waste forms
- Microbial Science research on areas such as bio-remediation and microbial transport
- Plant Science area such as phytoremediation
- Separations Chemistry that focuses on high level tank waste treatment alternatives.

DOCUMENT LAYOUT

This volume catelogues publications and other communications products from EMSP-funded research by EMSP Problem Area and Science Category, and includes the project number, title, name of the principal investigator, and a brief description of the respective project. Research transition activities, as well as projects success posters, fact sheets, and workshop summaries, are documented in *Research Accomplishments for the Envornmental Management Science Program*.

Communication Products. This section provides a list of publications by EMSP project. Journal articles, papers, reports, presentations, posters, and media reports are considered publications for the purposes of this summary. To date, 2001 communications products have resulted from EMSP funded research.

Transitions between Problem Areas are indicated by oversized, bold text on a shaded background, with associated science categories appearing as bold text preceded by a shaded horizontal rule, as follows.

EMSP Problem Area

EMSP Science Category

Photos and illustrations are placed throughout the document to coincide with information regarding the EMSP research project to which they apply.

Communications
Products

EMSP COMMUNICATION PRODUCTS

One of the goals of the EMSP is to focus the nation's science infrastructure on critical Department of Energy environmental problems. One of the "tried and true" ways to increase the general body of knowledge within the scientific community is through publication of research methods, results, and issues. EMSP research has provided a basis for numerous information exchanges through this method. EMSP researchers and staff have developed 2001 journal articles, papers, presentations, and other communication products. Many other news articles and press releases are either in development or planned as research within the program matures. The numbers of known publications and presentations as of October 31, 2001 are as follows:

674 Journal Articles
1 Media Report
45 Other (Encyclopedias, manuscripts)
38 Papers
37 Patent disclosures and applications
60 Posters
833 Presentations
6 Press Releases
185 Proceeding Contributions
68 Reports
54 Theses/Dissertations

NOTE: In instances where an author was not identified for a particular communication product, the lead principal investigator of the respective program has been listed as the author.

DEACTIVATION AND DECOMMISSIONING

Analytical Chemistry & Instrumentation

Project: 65001

Title: Development of Novel, Simple Multianalyte Sensors for Remote Environmental Analysis

PI: Dr. Sanford A. Asher *Institution:* University of Pittsburgh

Publication Type: Journal

Holtz, J. H. & Asher, S. A. (1997). Intelligent polymerized crystalline colloidal array hydrogel film chemical sensing materials. Nature. 389, 829-832.

Holtz, J. H., Holtz, J. S. W., Munro, C. H., & Asher, S. A. (1998). Intelligent polymerized crystalline colloidal arrays: Novel chemical sensor materials. Anal. Chem. 70, 780-791.

Holtz, J., Weissman, J., Pan, G., & Asher, S. A. (1998). Mesoscopically periodic photonic crystal materials for linear and nonlinear optics and chemical sensing. Material Research Soc. 23, 44-50.

Project: 65004

Title: Real-Time Identification and Characterization of Asbestos and Concrete Materials with Radioactive Contamination

PI: Dr. George Xu *Institution:* Rensselaer Polytechnic Institute

Publication Type: Journal

Naessens, E. P. & Xu, X. G. (1999). A non-destructive method to determine the depth of radionuclides in materials in-situ. Health Phys. 77(1), 76-88.

Publication Type: Presentation

Chen, Q., Jiang, Z., Sun, F. G., & Zhang, X. -C. (1999, May). Two-fold improvement of THz optoelectronic generation and detection. CLEO'99. Baltimore, MD.

Jiang, Z., Sun, F. G., Chen, Q., & Zhang, X. -C. (1999, May). Electro-optic sampling near zero optical transmission point. CLEO'99. Baltimore, MD.

Biogeochemistry

ORNL research, Cathy McKeown, working with depleted uranium and contaminated steel coupons. [see Project #64907]

Project: 64907

Title: "Green" Biopolymers for Improved Decontamination of Metals from Surfaces: Sorptive Characterization and Costing Properties

PI: Dr. Brian H. Davison

Institution: Oak Ridge National Laboratory

Publication Type: Poster

Davison, B. H. (1998, Nov. 17-18). Green biopolymers for decontamination. Poster presentation at Workshop on integration of end user needs with research projects for EMSP: Focus on Deactivation and Decommissioning at Savannah River Site.

Publication Type: Presentation

Preparation of Contaminated Steel Coupons. [see Project #64907]

Davison, B. H. (1999, Sept. 12-17). Green biopolymer for decon of contaminated surfaces. Decontamination, Demolition, and Restoration (DD&R) Topical Meeting on Site Restoration of Government and Commercial Facilities. Knoxville, TN.

Kuritz, T. (1999, Sep.). Remediation by cyanobacteria. International Meeting on Applied Algology, Monte Cantini Terme, Italy.

Project: 64931

Title: Microbially Promoted Solubilization of Steel Corrosion Products and Fate of Associated Actinides

PI: Dr. Yuri A. Gorby *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Das, A. & Caccavo, F. (2000). Dissimilatory Fe(III) oxide reduction by Shewnella alga BrY requires adhesion. Current Microbiology. 40(5), 344-347.

Das, A. & Caccavo, F. (2001). Adhesion of the dissimilatory Fe(III)-reducing bacterium Shewnnella alga BrY to cystalline Fe(III) oxides. Current Microbiology. 42(3), 151-154.

Engineering Science

Project: 55052

Title: Advanced Sensing and Control Techniques to Facilitate Semi-Autonomous Decommissioning

PI: Dr. Robert J. Schalkoff *Institution:* Clemson University

Publication Type: Journal

Costescu, N., Dawson, D., & Loffler, M. (1999, Jun.). Qmotor 2.0 - A real-time PC based control environment. IEEE Contr. Syst. Mag. 19(3), 68-76.

Costescu, N., Loffler, M., Zergeroglu, E., & Dawson, D. (1998, in press). Q robot - a multitasking PC based robot control system. Microcomputer Applications Journal Special Issue on Robotics.

Publication Type: Other

Geist, R., Schalkoff, R., Stinson, T., & Gurbuz, S., (1997). Autonomous virtualization of real environments for telepresence applications. PRESENCE: Teleoperators and Virtual Environments, 6,6. MIT Press, 645-657.

Publication Type: Proceeding

Costescu, N., Loffler, M., Zergeroglu, E., & Dawson, D. (1998, Sept.). Q robot: A Multitasking PC based robot control system. Proceedings of the IEEE Conference on Control Applications. Trieste, Italy. 892-896.

Geist, R., Vernon, D., & Schalkoff, R. (1998, Apr.). Rendering inversion in the automated construction of virtual environments. Proceedings of the 3rd ASCE Specialty Conf. on Robotics for Challenging Environments (ROBOTICS '98). Albuquerque, NM. 85-91.

Geist, R., Westall, J., Tregila, D., & Smotherman, M. (1998, Dec.). Real-time, 3-D graphics for the Linux PC. Proceeds of the 24th Annual Int. Conf. of the Computer Measurement Group (CMG98), Anaheim, CA. 863 - 873.

Van Pernis, A. (1999, Apr.). Surface construction from within a virtual environment. Proceedings of the Annual ACM Southeast Conference. Mobile, AL. NOTE: this was the winning paper in the ACM SE student paper competition.

Project: 64979

Title: Basic Engineering Research for D&D of R.Reactor Storage Pond Sludge: Electrokinetics, Carbon Dioxide Extraction, and Supercritical Water Oxidation

PI: Dr. Edward A. Hamilton *Institution:* SCUREF

Publication Type: Journal

Yang, X. -N., Coelho, L. A. F., & Matthews, M. A. (2000). Near-critical behavior of mutual coefficients for five solutes in supercritical carbon dioxide. Industrial & Engineering Chemistry Research. 39(8), 3059-3068.

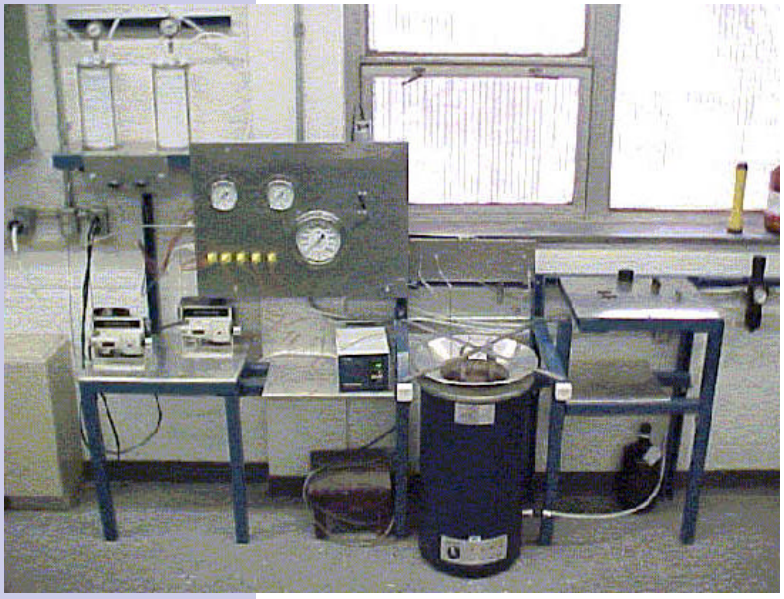
Publication Type: Poster

Bruce, D. (1998, Nov. 15-20). Sonochemical oxidation of organic contaminants in waste water. Presentation at the AIChE Annual Meeting. Miami Beach, FL.

Bruce, D. A., Nareddy, A. (1999, Nov. 3). Prediction of sonochemical oxidation rates for organic contaminants in water. AIChE National Meeting, Dallas, TX.

Leonard, M. L., Weidner, J. W., White, R. E., & Matthews, M. A. (1999, Sept. 26 - Oct. 1). Electrochemical reactions in supercritical fluids in materials processing and synthesis. Davos, Switzerland.

Matthews, M. (1998, Nov. 15-20). Mass transfer in CO2/surfactant systems. Presentation at the 1998 AIChE Annual Meeting. Miami Beach, FL.



Supercritical Water Oxidation Test Stand at Clemson University. [see Project #64979]

Matthews, M. A. (2000, Apr. 24-27). Basic engineering research for D&D of PCB wastes at DOE sites. Mixed Waste Focus Area Working Group, Environmental Management Science Program National Workshop, Atlanta, GA.

Matthews, M. A., Bruce, D., & Thies, M. (2000, Apr. 24-27). Decontamination and decommissioning of PCB sites at DOE: Extraction, electrokinetics, and hydrothermal oxidation. Environmental Management Science Program National Workshop, Atlanta, GA.

PIckett, J., et. al. (1998, Nov. 17-18). Decontamination and decommissioning

of PCB sites at SRS. Poster presentation at the Workshop on Integration of End User Needs with Research Projects for the Environmental Management Science Program. Savannah River Site. Aiken, SC.

Publication Type: Presentation

Bruce, D. A. & Nareddy, A. (2000, Nov.). Dynamics of sonochemical reactors. AIChE. Los Angeles, CA.

Bruce, D. A., Dolan, H., Nareddy, A., & Haseltine, E. (1999, Nov. 3). Diffusional effects on the sonochemical oxidation of organic contaminants in wastewater. AIChE Annual Meeting, Dallas, TX.

Extraction apparatus at University of South Carolina [Project #64979]

Hamilton, E. A. & Matthews, M. A. (2000, Apr. 24-27). Linking EMSP research to end-user's needs: A case study. Environmental Management Science Program National Workshop, Atlanta, GA.

Jun, L. & Matthews, M. A. (2000, Aug. 20-24). Supercritical CO2 extraction of chlorinated aromatics from job control waste. 2000 Annual Meeting of the American Chemical Society, Washington, D. C.

Leonard, M. L., Weidner, J. W., & Matthews, M. A. (2000, Sept. 3-8). Electrochemical reactions in supercritical carbon dioxide. 51st Annual Meeting of the International Society of Electrochemists. Warsaw, Poland.

Project: 65015

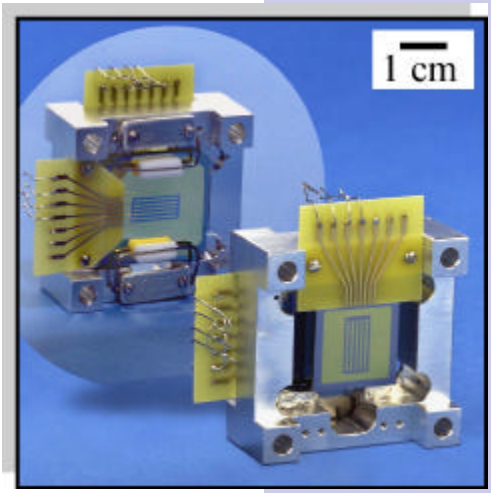
Title: Three-Dimensional Position-Sensitive Germanium Detectors

PI: Dr. Mark Amman

Institution: Lawrence Berkeley National Laboratory

Publication Type: Presentation

Amman, M. & Luke, P. N. (2000, Aug.). Position-sensitive germanium detectors for gamma-ray imaging and spectroscopy. Hard X-Ray, Gamma-Ray, and Neutron Detector Physics II Conference, SPIE Annual Meeting, San Diego, CA.



One of several small prototype position-sensitive germanium detectors fabricated for this project. Using such detectors, we have refined our detector fabrication process and developed techniques to improve both the imaging and spectroscopic performance of the detectors. [see Project #65015]

Amman, M., Luke, P. N., & Burks, M. T. (2000, Apr.). Three-dimensional position-sensitive germanium detectors. Environmental Management Science Program National Workshop, Atlanta, GA.

Publication Type: Report

Amman, M. & Luke, P. N. (2000). Position-sensitive germanium detectors for gamma-ray imaging and spectroscopy. Proceedings of SPIE, Hard X-Ray, Gamma-Ray, and Neutron Detector Physics II Conference. Lawrence Berkeley National Laboratory Report LBNL-45022.

Amman, M. & Luke, P. N. (2000). Three-dimensional position sensing and field shaping in orthogonalstrip germanium gamma-ray detectors. Nuclear Instruments and Methods in Physics Research A. 452, 155-166. Lawrence Berkeley National Laboratory Report LBNL-44898.

Luke, P. N., Amman, M., Phlips, B. F., Johnson, W. N., & Kroeger, R. A. (2000). Germanium orthogonal strip detectors with amorphous-semiconductor contacts. IEEE Transactions on Nuclear Science. Lawrence Berkeley National Laboratory Report LBNL-44444.

Project: 82773 (Renewal of Project No. 64947)

Title: Contaminant-Organic Complexes: Their Structure and Energetics in Surface Decontamination Processes

PI: Dr. Calvin C. Ainsworth *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Hay, B. P. & Hancock, R. D. (2001). The role of donor group orientation as a factor in metal ion recognition by ligands. Coord. Chem. Rev. 212, 61+.

Vargas, R., Garza, J., Dixon, D. A., & Hay, B. P. (2001). C(sp2)-C(aryl) bond rotation barrier in N-methylbenzamide. J. Phys. Chem. A. 105, 774-778.

Vargas, R., Garza, J., Dixon, D. A., & Hay, B. P. (2001, in press). Conformational analysis of N-benzylformamide. J. Mol. Struct. (THEOCHEM).

Publication Type: Presentation

Beak, D. G., Chen, C. C., Bigham, J. M., & Traina, S. J. (1999, Jun.). Synthesis and properties of hematite, maghematite, and their chromium substituted analogs. The Clay Minerals Society 36th Annual Meeting. Purdue University, IN.

Chen, C. C. & Traina, S. J. (2000, Apr.). Macrosopic and microscopic investigation of lanthanide ions partitioning at oxide/water surfaces. EMSP National Workshop. Atlanta, GA.

Chen, C. C. & Traina, S. J. (2001, May). Dissolution of iron oxides and Cr-substituted iron oxides with sorbed europium by the Siderophore Desferrioxamine B. Goldschmidt Conference. Hot Springs, VA.

Hay, B. P. (2000, Dec. 16). Building a better mousetrap: Ligand design with molecular mechanics. Invited presentation at the American Chemical Society Pacifichem 2000 Meeting. Honolulu, HI.

Hay, B. P. (2000, Mar. 23). Ligand design with molecular mechanics. Theory, Modeling, and Simulation Monthly Seminar Series. Richland, VA.

Hay, B. P. (2000, Mar. 26). Ligand design with molecular mechanics. 219th American Chemical Society Meeting. San Francisco, CA.

Hay, B. P., Vargas, R., Garza, J., & Dixon, D. A. (2000, Mar. 26). Metal ion complementarity in a series of Tris-Catecholamides. 219th American Chemical Society Meeting. San Francisco, CA.

Traina, S. J. & Chen, C. C. (2000, Sept.). XAS investigation of lanthanide ion sorption on iron oxide and Cr-substituted iron oxide surfaces. Goldschmidt Conference. Oxford, UK.

Inorganic Chemistry

Project: 54724

Title: Synthesis of New Water-Soluble Metal-Binding Polymers: Combinatorial Chemistry Approach

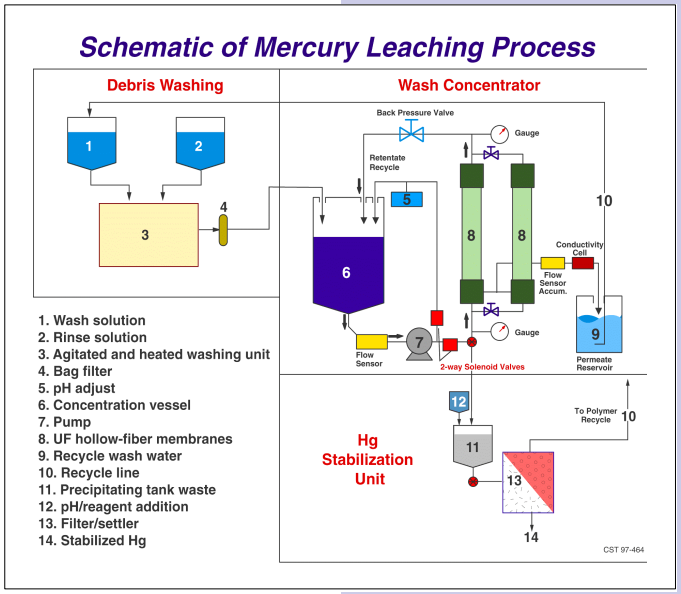
PI: Dr. Barbara F. Smith *Institution:* Los Alamos National Laboratory

Publication Type: Journal

Colletti, L. & Havrilla, G. (1999). Trace element detection with micro-x-ray fluorescence. Advances in X-Ray Analysis, 44.

Corrales, L. R., Song, J., & Van Ginhoven, R. (1999, Mar. 21). The formation and migration energetics of radical defects in silica polymorphs. Abstr. Pap. Am. Chem. S. 217, U293-U293, Part 2.

Kizer, D. E., Miller, R. B., & Kurth, M. J. (1999). Fused pyrazolo heterocycles: intramolecular [3+2]-nitrile oxide cycloadditions applied to syntheses of pyrazolo[3,4-g][2,1]dihydrobenzoisoxazol(in)es. Tetrahedron Letters. 40, 3535-38.



Schematic of Groundwater and Soil Remediation Process [see Project #54724]

Publication Type: Proceeding

Smith, B. F., Robison, T. W., & Jarvinen, G. D. (1998). Water-soluble metal-binding polymers with ultrafiltration: A technology for the removal, concentration, and recovery of metal ions from aqueous streams. Rogers, R., Bond, A., & Dietz, M. (Eds.), ACS Symposium Series volume, Advances in Metal Ion Separation and Preconcentration, Chap. 20, 294-330.

Song, J., Corrales, L. R., & Jónsson, H. (1999, in press). Exploring the excited states of vacancy defects in silica. Zinkle, S. J., Ewing, R. C., Lucas, G. E., & Williams, J. S. (Eds.), Microstructural Processes in Irradiated Materials. Mater. Res. Soc. Symp. Proc. 540, Warrendale, PA.

Materials Science

Project: 55380

Title: In-Situ Spectro-Electrochemical Studies of Radionuclide Contaminated Surface Films on Metals and the Mechanism of their Formation and Dissolution

PI: Dr. Carlos A. Melendres *Institution:* Argonne National Laboratory

Publication Type: Journal

Balasubramanian, M. & Melendres, C. A. (1999). An x-ray absorption near-edge spectroscopy study of the oxidation state of chromium in electrodeposited oxide films. Electrochim. Acta. 44, 2941.

Balasubramanian, M. & Melendres, C. A. (1999). Selective site occupancy exhibited by Cr3+ and Cr6+ incorporated into electrochemically deposited nickel hydroxide films. Electrochem. and Solid State Lett. 2, 167.

Balasubramanian, M., Melendres, C. A., & Mansour, A. N. (1999). X-ray absorption spectroscopy study of the local structure of heavy metal ions incorporated into electrodeposited nickel oxide films. J. Electrochem. Soc. 146, 607.

Balasubramanian, M., Melendres, C. A., Mansour, A. N., & Mini, S. (1999). X-ray absorption spectroscopy studies of electrochemically deposited thin oxide films. Mater. Res. Symp. Proc. 524.

Wang, H., et. al. (1998). Integrated x-ray L absorption spectra: Counting holes in Ni complexes. J. Phys. Chem. B 102, 8343.

Publication Type: Paper

Carlos, A. (1999, Apr. 5). X-ray absorption spectroscopy studies of electrochemically deposited thin oxide films. Materials Research Society Spring Meeting.

Melendres, C. A. (1999, May 3). X-ray absorption spectroscopy studies of the structure of electrodeposited metal oxide films and some applications. 193rd Meeting of the Electrochemical Society.

Publication Type: Presentation

Balasubramanian, M. & Melendres, C. A. (1999). Local structure of chromium incorporated into electrodeposited nickel hydroxide films. J. Synchrotron Radiat. 6, 594.

Balasubramanian, M., Melendres, C. A., & Mansour, A. N. (1999). An x-ray absorption study of the local structure of cerium in electrochemically deposited thin films. Thin Solid Films. 347, 178.

Project: 59925

Title: Modeling of Diffusion of Plutonium in Other Metals and of Gaseous Species in Plutonium-Based Systems

PI: Dr. Bernard R. Cooper *Institution:* West Virginia University

Publication Type: Journal

Cooper, B. R., Becker, J. D., Wills, J. M., & Cox, L. (1998). Calculated lattice relaxation in Pu-Ga alloys. Journal of Alloys and Compounds. 271-273, 367.

Cooper, B. R., Becker, J. D., Wills, J. M., & Cox, L. (1998). Calculated lattice relaxation in Pu-Ga. Phys. Rev. B. 58B, 5143.

Cooper, B. R., Vogt, O., Sheng, Q.G., & Lin, Y.L. (1999, May). From heavy fermions to random-localized-site behavior via Anderson localization. Philosophical Magazine B 79. No. 5, 683-702.

Publication Type: Other

Cooper, B. R., Turchi, P.E.A., Gonis, A., Kioussis, N., & Price, D. L. (1999). Correlation effects on stability in Pu metal and its alloys. Gonis, A. & Kioussis, N. (Eds.), Electron Correlations and Materials Properties. Plenum Publishing.

Publication Type: Presentation

Cooper, B. R. & Beiden, S. (1998). Diffusion of plutonium into transition metallic alloys and of transition metal species into plutonium. Eighth Conference on Computational Research on Materials. Lakeview, WV.

Cooper, B. R. & Beiden, S. (1998). Modeling of diffusion of plutonium in other metals and of gaseous species in plutonium-based systems. Environmental Management Science Workshop. Chicago, IL.

Cooper, B. R. & Beiden, S. (1998, Nov.). Modeling of diffusion of plutonium. Workshop on Environmental Management Science: Integration with End User Needs. Savannah River Site. Aiken, SC.

Cooper, B. R. & Beiden, S. (1998, Nov.). Modeling of interdiffusion of plutonium and other metals. Materials Research Society Meeting. Boston, MA.

Cooper, B. R. & Lederman, D. (1998, Nov.). Portable detection and analysis of plutonium content. Workshop on Environmental Management Science: Integration with End User Needs. Savannah River Site. Aiken, SC.

Cooper, B. R. (1998, Jun. 28 - Jul. 3). Synthesis of many-body theory and electronic structure. International Workshop on Electron Correlations and Materials Properties. Heraklion, Crete, Greece.

Cooper, B. R. (1998, May). Treating electronic and magnetic properties of actinide-based materials beyond one-electron dynamics. School of Actinide Physics and Chemistry. Uppsala, Sweden.

Cooper, B. R. (1999, Apr.). Random 5f localization and the fcc transition and depression of melting temperature in plutonium. 29th Journees des Actinides Conference. Luso, Portugal.

Cooper, B. R. (1999, Mar.). Anomalous electronic behavior and relationship to thermostructural behavior of light actinides. American Physical Society Meeting. Atlanta, GA.

Cooper, B. R., Becker, J. D., Wills, J. M. & Cox, L. (1997, Sept.). Structural relaxation in Pu-Ga via full-potential LMTO calculations. Actinides 97. International Conference. Baden-Baden, Germany.

Cooper, B. R., Kioussis, N., Turchi, P. E. A., Gonis, A., & Price, D. L. (1999, Mar.). Electronic structure of alpha and delta plutonium. American Physical Society Meeting. Atlanta, GA.

Cooper, B. R., Sevilla, E. H., & Fernando, G. W. (1999, Mar.). Equilibrium lattice volume of fcc Pu. American Physical Society Meeting. Atlanta, GA.

Project: 64896

Title: Decontamination of Radionuclides from Concrete During and After Thermal Treatment

PI: Dr. Brian P. Spalding *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Spalding, B. (2000). Simple heating of contaminated cement paste between 800-1300°C can lead to complete volatilization of 137Cs making its facile decontamination from concrete a feasible remedial technique. Environ. Sci. Technol. 34, 5051-5058.

Spalding, B. P. (2000, in press). A chemical equilibria model of strontium-90 adsorption and movement in soil under dynamic alkaline conditions. Environmental Science & Technology.

Spalding, B. P. (2000, in press). Volatility and extractability of cesium-134, strontium-85, cobalt-57, and uranium after heating hardened portland cement paste. Environmental Science & Technology.

Publication Type: Presentation

Spalding, B. P. (1998, Nov. 17-18). Decontamination of radionuclides from concrete during and after thermal treatment. Workshop on Integration of End User Needs with Research Projects for Environmental Management Science Program, Savannah River Site, Aiken, SC.

Spalding, B. P. (1999, Jan. 13). Is it a good idea to heat radioactively-contaminated concrete or soil? Civil Engineering Dept., Northwestern University, Evanston, IL.

Spalding, B. P. (1999, Sep. 22). Decontamination of radionuclides from concrete during and after thermal treatment. U. S. Dept. of Energy - Oak Ridge Operations, Environmental Management Science Program National Workshop, Oak Ridge, TN.

Spalding, B. P. (2000, Apr. 24). Decontamination of radionuclides from concrete during and after thermal treatment. 2nd Annual Environmental Management Science Program National Workshop, Atlanta, GA.

Project: 64946

Title: Mechanisms of Radionuclide-Hydroxycarboxylic Acid Interactions for Decontamination of Metallic Surfaces

PI: Dr. Arokiasamy J. Francis *Institution:* Brookhaven National Laboratory

Publication Type: Presentation

Halada, G. P., et. al. (1999, May 2-6). Interaction of uranium with corrosion products formed on plain carbon steel. Paper presentation at the 195th Meeting of the Electrochemical Society. Seattle, WA.

Publication Type: Proceeding

Francis, A. J., Dodge, C. J., Gillow, J. B., Halada, G. B., & Clayton, C. R. (1999, Aug. 22-26). Decontamination of uranium contaminated metallic surfaces with uranium recovery. Paper presentation NUCL-65 at the Symposium on First Accomplishments of Environmental Management Science Program, 218th Annual Meeting of the American Chemical Society. New Orleans, LA.

Halada, G. P., et. al. (1999, Aug. 22-26). A spectroscopic study of the association of contaminant uranium with mild steel corrosion products. Paper presentation NUCL-61at the Symposium on First Accomplishments of Environmental Management Science Program, 218th Annual Meeting of the American Chemical Society. New Orleans, LA.

Project: 73835 (Renewal of Project No. 54914)

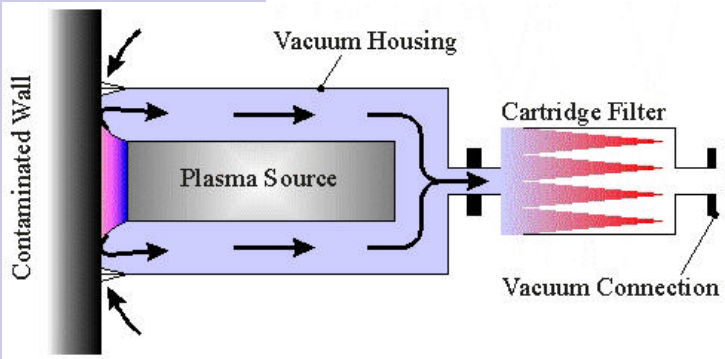
Title: Atmospheric-Pressure Plasma Cleaning of Contaminated Surfaces

PI: Dr. Robert F. Hicks *Institution:* University of California at Los Angeles

Publication Type: Journal

Babayan, S. E., et. al. (1998, Aug.). Deposition of silicon dioxide films with an atmospheric-pressure plasma jet. Plasma Sources Sci. T. 7(3), 286-288.

Babayan, S. E., et. al. (1998, in press). Plasma source science and technology.



Schematic of a method for decontaminating surfaces, such as building wall. The plasma source is mounted within a housing that keeps the pressure slightly below ambient to prevent the etch products from escaping the device. A cartridge filter for the radioactive contaminants can be placed near the plasma source and replaced periodically as needed. [see Project #73835, renewal of #54914]

Babayan, S. E., Jeong, J. Y., Tu, V. J., Selwyn, G. S., & Hicks, R. F. (1998). Deposition of glass films with an atmospheric-pressure plasma jet. Plasma Sources Sci. and Tech. 7, 286-288.

Jeong, J. Y., et. al. (1998, Aug.). Etching materials with an atmospheric-pressure plasma jet. Plasma Sources Sci. T. 7(3), 282-285.

Jeong, J. Y., et. al. (1999, Sep.-Oct.). Etching polymide with a non-equilibrium atmospheric-pressure plasma jet. J. Vac. Sci. Technol. A. 17(5), 2581-2585.

Park, J., et. al. (2000, in press). An atmospheric pressure plasma source. Appl. Phys. Lett.

Schutze, A., et. al. (1998, Dec.). The atmospheric-pressure plasma jet: A review and comparison to other plasma sources. IEEE T. Plasma Sci. 26(6), 1685-1694.

Side view of a 4" wide atmospheric-pressure plasma source operating with 750 Torr helium and 10 Torr oxygen. [see Project #73835, renewal of #54914]

Publication Type: Patent

Selwyn, G. S. (1999, Oct. 5). Atmospheric-pressure plasma jet. US #5,961,772.

Publication Type: Presentation

Henins, I., Selwyn, G. S., Park, J., Snyder, H., & Herrmann, H. (1999, Mar. 31). The atmospheric pressure plasma jet (2 presentations, Parts A & B). New Mexico Chapter Meeting of the American Vacuum Society, Albuquerque, NM.

Hicks, R. F. (1998, Feb. 27). Materials processing with atmospheric-pressure plasma jets. Solid State Technology and Devices Seminar, Electrical Engineering and Computer Sciences Department, University of California, Berkeley, CA.

Hicks, R. F. (1999, Feb. 1). Materials processing with atmospheric-pressure plasma jets. Université D'Orléans, France.

Hicks, R. F., Babayan, S. E., Jeong, J. Y., Henins, I., & Selwyn, G. S. (1998, Jun. 2). Atmospheric-pressure plasma jet processing of materials. The 25th International Conference on Plasma Science, Raleigh, NC.

Hicks, R. F., Babayan, S. E., Jeong, J. Y., Henins, I., & Selwyn, G. S. (1997, Sep.). Atmospheric-pressure plasma jet processing of materials. ISAPS Conference, Los Angeles, CA.

Hicks, R. F., et. al. (1998, Nov. 17). Characterization of the atmospheric pressure plasma jet effluent. AIChE Annual Meeting, Miami, FL.

Hicks, R. F., et. al. (1999, Nov. 2). Gas-phase chemistry of atmospheric pressure plasmas. AIChE Annual Meeting. Dallas, TX.

Jeong, J. Y., Babayan, S. E., Selwyn, G. S., & Hicks, R. F. (1997, Oct. 20). Atmospheric-pressure plasma jet etching of materials. 44th International Symposium of the American Vacuum Society, San Jose, CA.

Jeong, J. Y., et. al. (1997, Nov. 19). Atmospheric-pressure plasma jet etching of materials. AIChE Annual Meeting, Los Angeles, CA.

Jeong, J. Y., et. al. (1998, Nov. 5). Characterization of the reactive species in a helium/oxygen atmospheric-pressure plasma jet. 45th International Symposium of the American Vacuum Society, Baltimore, MD.

Schuetze, A., Babayan, S. E., Jeong, J. Y., Tu, V. J., & Hicks, R. F. (1998, Nov. 18). Atmospheric-pressure plasma cleaning of Si(100) surfaces. AIChE Annual Meeting, Miami, FL.

Schuetze, A., et. al. (1998, Nov. 4). The atmospheric-pressure plasma jet: Properties and materials applications. 45th International Symposium of the American Vacuum Society, Baltimore, MD.

Selwyn, G. S. (1998, May 5). Cleaning and decontamination using the atmospheric pressure plasma jet. International Science and Technology Conference, Albuquerque, NM.

Selwyn, G. S., et. al. (1997, Nov. 17). Contamination control for future device processing: Good vibrations to plasma jets. AIChE Annual Meeting, Los Angeles, CA.

Selwyn, G. S., Henins, I., Jeong, J. Y., Babayan, S. E., & Hicks, R. F. (1997, Oct. 22). High rate cleaning of surfaces using atmospheric pressure generation of reactive metastable species. American Vacuum Society Annual Meeting, San Jose, CA.

Selwyn, G. S., Henins, I., Park, J., Snyder, H., & Herrmann, H. (1999, Feb. 24). The atmospheric pressure plasma jet. IPEC-Precision, Bethel, CT.

Selwyn, G. S., Henins, I., Park, J., Snyder, H., & Herrmann, H. (1999, Mar. 18). The atmospheric pressure plasma jet. Watkins-Johnson, Scotts Valley, CA.

Separations Chemistry

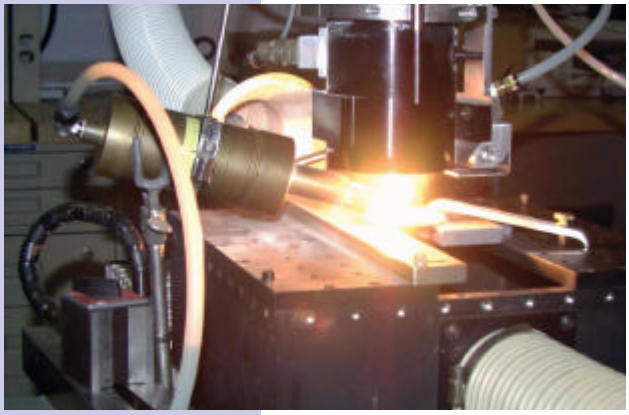
Project: 60283

Title: Waste Volume Reduction Using Surface Characterization and Decontamination by Laser Ablation

PI: Dr. Michael J. Pellin *Institution:* Argonne National Laboratory

Publication Type: Journal

Savina, M., Xu, Z. Y., Wang, Y., Pellin, M., & Leong, K. (1999, Dec.). Pulsed laser ablation of cement and concrete. J. Laser Appl. 11(6), 882-886.



Laser Ablation System – 1.6 kw pulsed Nd:YAG laser system with fiber optic beam delivery. Advantages of this system over conventional scabbling are for hard-to-reach places and remote decontamination. [see Project #60283]

Publication Type: Poster

Savina, M. R., Pellin, M. J., Leong, K., & Xu, Z. (1998, Jul.). Waste volume reduction using surface characterization and decontamination by laser ablation. Presentation at EMSP Workshop. Rosemont, IL.

Publication Type: Presentation

Pellin, M. J., Savina, M. R., Reed, C. B., Wang, Y., & Xu, Z. (1999, Mar.). Waste volume reduction using surface characterization and decontamination by laser ablation. Presentation at Characterization, Monitoring, and Sensing Workshop. Gaithersburg, MD.

Publication Type: Proceeding

Savina, M. R., Xu, Z., Wang, Y., Leong, K., & Pellin, M. J. (1998). Laser ablation of concrete. Proceedings of the 17th International Conference on Applications of Lasers and Electro-Optics. 85A, 219-226.

Project: 64912

Title: Improved Decontamination: Interfacial, Transport, and Chemical Properties of Aqueous Surfactant Cleaners

PI: Dr. David W. DePaoli *Institution:* Oak Ridge National Laboratory

Publication Type: Presentation

Counce, R. M. (1999, Nov. 17-18). Improved decontamination: Interfacial, transport, and chemical properties of aqueous surfactant cleaners. Presentation at the EMSP/D&D Workshop, Savannah River Site, Aiken, SC.

DePaoli, D. W., Hu, M. Z., Counce, R. M., & Rowe, A. W. (1999, Nov. 30). Overview of improved decontamination: Interfacial, transport, and chemical properties of aqueous surfactant cleaners. Presentation at the DOE Oak Ridge Operations D&D Focus Area Site Visit, Oak Ridge, TN.

DePaoli, D. W., Hu, M. Z., Counce, R. M., & Rowe, A. W. (2000, Apr. 26). Surface decontamination with aqueous-based surfactant solutions. Presentation at the 2nd Annual Environmental Management Science Program National Workshop, Atlanta, GA.

DePaoli, D. W., Hu, M. Z., Rowe, A. W., & Counce, R. M. (1999, Sep. 22). Improved decontamination: Interfacial, transport, and chemical properties of aqueous surfactant cleaners. Presentation at the Oak Ridge Operations Environmental Management Science Program Workshop, Oak Ridge, TN.

DePaoli, D. W., Hu, M. Z., Rowe, A. W., & Counce, R. M. (2000, Nov. 15). Surface cleaning with aqueous-based surfactant solutions. Presentation at the annual meeting of Chemical Engineers, Los Angeles, CA.

Perkins, L. W., Counce, R. M., Hu, M. Z.- C., & DePaoli, D. W. (1999, Oct. 17-21). Separation of oil from prototypic industrial cleaning/degreasing effluents. Eleventh Symposium on Separation Science and Technology for Energy Applications, Gatlinburg, TN.

Rowe, A. W., Counce, R. M., Hu, M. Z.- C., & DePaoli, D. W. (1999, Oct. 17-21). Surface decontamination with aqueous-based surfactant solutions. Eleventh Symposium on Separation Science and Technology for Energy Applications, Gatlinburg, TN.

Publication Type: Theses/Dissertations

Morton, S. (in progress). Improved decontamination: Interfacial, transport, and chemical properties of aqueous surfactant cleaners. PhD. Dissertation, University of Tennessee, Knoxville, TN.

Rowe, A. W. (2000, Aug.). Improved decontamination: Interfacial, transport, and chemical properties of aqueous surfactant cleaners. M. S. Thesis, University of Tennessee, Knoxville, TN.

Project: 64965

Title: Supercritical Carbon Dioxide-Soluble Ligands for Extracting Actinide Metal Ions from Porous Solids

PI: Dr. Mark L. Dietz *Institution:* Argonne National Laboratory

Publication Type: Journal

Griffith-Dzielawa, J. A., Barrans, R. E., McAlister, D. R., Dietz, M. L., & Herlinger, A. W. (2000). Synthesis and characterization of di-[3-(trimethylsilyl)1-propylene] alkylenediphosphonic acids. Synthetic Commun. 30(12), 2121-2132.

Publication Type: Poster

Herlinger, A. W., Griffith, J. A., McAlister, D. R., & Barrans Jr., R. E. (1999, Aug. 22-26). Functionalized diphosphonic acid ligands for metal ion coordination in supercritical carbon dioxide. Poster presentation #33 at the First Accomplishments of the Environmental Management Sciences Program Symposium sponsored by the Division of Nuclear Chemistry and Technology at the 218th National A.C.S. Meeting. New Orleans, LA.

HEALTH/ECOLOGY/RISK

Analytical Chemistry & Instrumentation

Project: 60163

Title: Investigation of Techniques to Improve Continuous Air Monitors Under Conditions of High Dust Loading in Environmental Settings

PI: Dr. Stephen D. Schery *Institution:* New Mexico Institute of Mining & Technology

Publication Type: Presentation

Rodgers, J. C., Wasiolek, P. T., Schery, S. D., & Alcantara, R. E. (1998, Nov. 1-6). High resolution real-time optical studies of radiological air sample processes in an environmental continuous air monitor. 1998 SPIA Symposium on Industrial and Environmental Monitors and Biosensors. Boston, MA. LA-UR-98-1684.

Project: 60474

Title: Ultrahigh Sensitivity Heavy Noble Gas Detectors for Long-Term Monitoring and Monitoring Air

PI: Dr. John D. Valentine *Institution:* Georgia Institute of Technology

Publication Type: Journal

Valentine, J. D. (1999). Evaluating detectors and pulse processing techniques. IEEE Transactions in Nuclear Science. 46(3).

Publication Type: Other

Valentine, J. D. (1999). Small prototype fluid transfer system and its performance. Nuclear Instruments and Methods in Physics Research, Section A. 422, 820-825.

Project: 73807 (Renewal of Project No. 60218)

Title: Rapid Nucleic Acid Analysis for Contaminant Evaluation

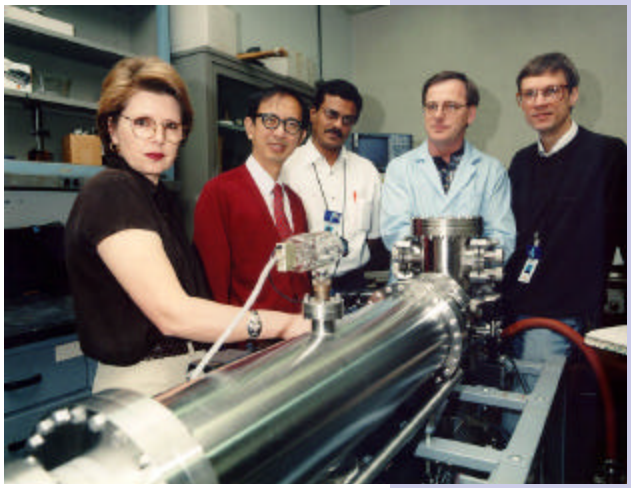
PI: Dr. Chung H. Chen *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Chen, C. H., et. al. (1999). Laser desorption mass spectrometry for high throughput DNA analysis and its applications. SPIE Int. Soc. Opt. Eng. 3602, 338-345.

Golovlev, V. V., Allman , S. L., Garrett, W. R., Taranenko, N. I., & Chen, C. H. (1997). Laser induced acoustic desorption. International Journal of Mass Spectrometry and Ion Processes. 169/170, 69-78.

Isola, N. R., Allman, S. L., Golovlev, V. V., & Chen, C. H. (1999). Chemical cleavage sequencing of DNA using matrix-assisted laser desorption/ionization time-of-flight mass spectrometry. Analytical Chemistry. 71, 2266-2269.



Researchers working to develop the new DNA detection technology by using laser induced acoustic desorption mass spectrometry. [see Project #73807, renewal of #60218]

Taranenko, N. I., et. al. (1998). Matrix-assisted laser desorption/ionization for short tandem repeat loci. Rapid Comm. Mass Spectrom. 12, 413-418.

Taranenko, N. I., et. al. (1998). Sequencing DNA using mass spectrometry for ladder detection. Nucleic Acids Research. 26(10), 2488-2490.

Taranenko, N. I., Potter, N. T., Allman, S. L., Golovlev, V. V., & Chen, C. H. (1999). Detection of trinucleotide expansion by matrix-assisted laser desorption/ ionization time-of-flight mass spectrometry. Genetic Analysis. 15, 25-31.

Publication Type: Presentation

Chen, C. H. (1999, Mar. 26). Laser desorption mass spectrometry for rapid nucleic acid analysis. American Physical Society Centennial Meeting.

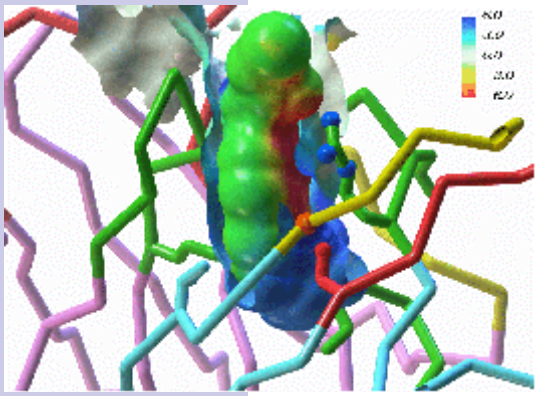
Health/Risk

Project: 54546

Title: Engineered Antibodies for Monitoring of Polynuclear Aromatic Hydrocarbons

PI: Dr. Alexander E. Karu *Institution:* University of California at Berkeley

Publication Type: Journal



A University of California project is using genetic engineering to improve detection of polynuclear aromatic hydrocarbons in the environment. [Project #54546]

Guo, F., Li, Q. X., & Alcantara-Licudine, J. P. (1999). A simple Na4 EDTA-assisted sub/supercritical fluid extraction procedure for quantitative recovery of polar analytes in soil. Anal. Chem. 71, 1309-1315.

Li, K., Chen, R., Zhao, B., Liu, M., Karu, A. E., Roberts, V. A., & Li, Q. X. (1999). Monoclonal antibody-based enzyme-linked immunosorbent assays for part-per-billion determination of polycyclic aromatic hydrocarbons: Effects of haptens and formats on sensitivity and specificity. Anal. Chem. 71, 302-309.

Liu, M., Li, Q. X, & Rechnitz, G. A. (1999). Flow injection immunosensing of polycyclic aromatic hydrocarbon with a quartz crystal microbalance. Analyt. Chim. Acta. 387, 29-38.

Liu, M., Li, Q. X, & Rechnitz, G. A. (2000, Jan). Gold electrode modification with thiolated hapten for the design of amperometric and piezoelectric immunosensors. Electroanal. 12(1), 21-26.

Liu, M., Rechnitz, G. A., Li, K. & Li, Q. X. (1998). Capacitive immunosensing of polycyclic aromatic hydrocarbon and protein conjugates. Anal. Lett. 31, 2025-2038.

Thomas, S. & Li, Q. X. (2000, Jun. 15). Immunoaffinity chromatography for the analysis of polycyclic aromatic hydrocarbons in corals. Environ. Sci. Technol. 34(12), 2649-2654.

Publication Type: Poster

Karu, A. E., Li, Q. X., & Roberts, V. (1998, July 27-30). Engineered antibodies for monitoring of polynuclear aromatic hydrocarbons. Poster presented at Department of Energy Environmental Science Management Program Workshop. Chicago, IL. http://www.doe.gov/em52/1998posters/id54546.pdf.

Publication Type: Presentation

Li, Q. X., Li, K., Thomas, S. & Li, H. (1999, Aug. 22-26). Application of immunochemical methods for the analysis of polynuclear aromatic hydrocarbons in the environment (Abstract No. NUCL0047). Symposium on First Accomplishments of the Environmental Management Science Program, 218th National Meeting of the American Chemical Society. New Orleans, LA.

Pellequer, J.-L., Zhao, B., Kao, H.-I., Karu, A. E., & Roberts, V. A. (1999, Aug. 22-26). Cation-pi interactions in antibody binding of polynuclear aromatic hydrocarbons (Abstract No. 36750). Symposium on First Accomplishments of the Enviironmental Management Science Program, ACS Div. of Nuclear Chemistry and Technology, 218th National Meeting of the American Chemical Society. New Orleans, LA.

Project: 54584

Title: Comparison of the Bioavailability of Elemental Waste Laden Soils Using in vivo and in vitro Analytical Methodology, and Refinement of Exposure/Dose Models

PI: Dr. Paul J. Lioy *Institution:* Univ of Medicine & Dentistry of NJ

Publication Type: Presentation

Ellickson, K. M., Kosson, D., Schopfer, C., & Lioy, P. J. (1999, Sep. 4-9). The bioaccessibility of radionuclides in contaminated soils using “in vitro” methods for the digestive system. Presentation at the 9th Annual Meeting of the International Society of Exposure Analysis. Athens, Greece.

Project: 54684

Title: Mechanism Involved in Trichloroethylene-Induced Liver Cancer: Importance to Environmental Cleanup

PI: Dr. Brian D. Thrall *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Bull, R. J. (2000, May). Mode of action of liver tumor induction by trichloroethylene and its metabolites, trichloroacetate, and dichloroacetate. Environ. Health Persp. 108, 241-259, Suppl. 2.

Kato-Weinstein, J., Lingohr, M. K., Thrall, B. D., & Bull, R. J. (1998). Effects of dichloroacetate on carbohydrate metabolism in B6C3F1 mice. Toxicology. 130, 141-154.

Lingohr, M. K., Thrall, B. D., & Bull, R. J. (1999, in press). Serum insulin levels and differential insulin receptor expression in livers and liver tumors of mice treated with dichloroacetate (DCA). Toxicol. Appl. Pharmacol.

Merdink, J. L., Gonzalez-Leon, A., Bull, R. J., & Schultz, I. R. (1998). The extent of dichloroacetate formation from trichloroethylene, chloral hydrate, trichloroacetate, and trichloroethanol in B6C3F1 mice. Toxicological Sciences. 45, 33-41.

Miller, J. H., et. al. (2000, Apr. 14). In vivo MRI measurements of tumor growth induced by dichloroacetate: Implications for mode of action. Toxicology. 145(2-3), 115-125.

Mounho, B. J. & Thrall, B. D. (1999, Sept. 1). The extracellular signal-regulated kinase pathway contributes to mitogenic and antiapoptic effects of peroxisome proliferations in vitro. Toxicol. Appl. Pharm. 159(2), 125-133.

Schultz, I. R., Merdink, J. L., Gonzalez-Leon, A., & Bull, R. J. (1999, Jul. 15). Comparative toxicokinetics of chlorinated and brominated haloacetates in F344 rats. Toxicol. Appl. Pharm. 158(2), 103-114.

Stauber, A. J., Bull, R. J., & Thrall, B. D. (1998). Dichloroacetate and trichloroacetate promote clonal expansion of anchorage-independent hepatocytes, in vivo and in vitro. Toxicol. Appl. Pharmacol. 150, 287-294.

Publication Type: Poster

Bull, R. J., Minard, K., Sasser, L.B., Lingohr, M. K., & Wind, R.A. (1999). Dichloroacetate-induced liver tumors cease growing on removal of treatment: Result of an insulin-sensitive phenotype? AACR Proceedings. 40, 3321

Publication Type: Presentation

Gonzalez-Leon, A., Merdink, J. L., Schultz, I. R., & Bull, R. J. (1998). Dichloroacetate auto-inhibits its degradation in the cytosol. Society of Toxicology, 37th Annual Meeting #426.

Kato-Weinstein, J., Thrall, B. D., & Bull, R. J. (1998). The effect of haloacetates on carbohydrate metabolism in B6C3F1 mice. Society of Toxicology, 37th Annual Meeting #308.

Lingohr, M. K., Thrall, B. D., & Bull, R. J. (1998). Dichloroacetate (DCA) affects proteins involved in insulin signaling in mouse liver cells. Society of Toxicology, 37th Annual Meeting #61.

Merdink, J. L., Schultz, I. R., & Bull, R. J. (1998). Formation of dichloroacetic acid in B6C3F1 mice from trichloroethylene or its metabolites. Society of Toxicology, 37th Annual Meeting #1621.

Mounho, B. J. & Thrall, B. D. (1998). Tumor promotion by peroxisome proliferators may involve the activation of mitogenic activated protein kinases (ERK1/ERK2). Society of Toxicology, 37th Annual Meeting #51.

Orner, G. A., et. al. (1998). Effects of trichloroacetate (TCA) and dichloroacetate (DCA) on H-ras in male B6C3F1 mice. Society of Toxicology, 37th Annual Meeting #60.

Schultz, I. R., Gonzalez-Leon, A., Merdink, J. L., & Bull, R. J. (1998). Comparative toxicokinetics and metabolism of halo-acetic acids in F344 rats. Society of Toxicology, 37th Annual Meeting #1045.

Stauber, A. J., Bull, R. J., & Thrall, B. D. (1998). Dichloroacetate and trichloroacetate promote clonal expansion of anchorage-independent hepatocytes. Society of Toxicology, 37th Annual Meeting #62.

Publication Type: Proceeding

Bull, R. J., Minard, K., Sasser, L. B., Lingohr, M. K., & Wind, R. A. (1999). Dichloroacetate-induced liver tumors cease growing on removal of treatment: Result of an insulin-sensitive phenotype? AACR Proceedings. 40, 3321.

Project: 55100

Title: Human Genetic Marker for Resistance to Radiations and Chemicals
PI: Dr. Howard B. Lieberman *Institution:* Columbia University

Publication Type: Journal

Hang, H., Rauth, S. J., Hopkins, K. M., Davey, S. K., & Lieberman, H. B. (1998). Molecular cloning and tissue-specific expression of Mrad9, a murine orthologue of the Schizosaccharomyces pombe rad9+ checkpoing control gene. J. Cell Physiol. 177, 232-240.

Project: 55356

Title: Environmentally-Induced Malignancies: An In Vivo Model to Evaluate the Health Impact of Chemicals in Mixed Waste
PI: Dr. Maria Pallavicini *Institution:* University of California at San Francisco

Publication Type: Journal

Giver, C. R., Moore II, D. H., & Pallavicini, M. G. (1999, Dec.). Radiation-induced translocation biomarkers: Assumptions tested using inbred mice with varying cancer predisposition. American Society of Hematology Meeting, New Orleans, LA.

Giver, C. R., Wong, R., Moore II, D. H., & Pallavicini, M. G. (2000, in press). Radiation-induced translocation biomarkers in inbred mice with varying cancer predisposition. Radiation Res.

Publication Type: Proceeding

Wong, R., Giver, C. R., & Pallavicini, M. (1999, Dec. 3-7). Benzene-induced toxicity and aneusomy in murine bone marrow hemopoietic stem cells. American Society of Hematology Meeting. New Orleans, LA.

Wong, R., Giver, C. R., & Pallavicini, M. (1999, Sep.). Benzene-induced toxicity and aneusomy in murine bone marrow hemopoietic stem cells. NIEHS Meeting - The Role of Human Exposure Assessment in the Prevention of Environmental Disease. Rockville, MD.

Project: 55410

Title: Determining Significant Endpoints for Ecological Risk Analysis

PI: Dr. Thomas G. Hinton *Institution:* Savannah River Ecology Laboratory

Publication Type: Journal

Congdon, J. D., Dunham, A. E., Hopkins, W. A., Rowe, C. L., & Hinton, T. G. (2000, in press). Resource-allocation based life histories: A conceptual basis for studies of ecologoical toxicology. Environmental Toxicology and Chemistry.

We are using an array of 50 outdoor mesocosms to address ecological risk questions. The mesocosm facility allows us to conduct replicated, controlled dose-effect studies on biota under continuous low-level exposure conditions. This photo shows thermoluminescent dosimeters placed within a mesocosm to test the homogeneity of the radiation exposure field. [see Project #55410]

Mülhlmann-Díaz, M. C., et. al. (2000, in press). Conservation of chromosome-1 in turtles over 66million years. Cytogenics and Cell Genetics.

Ulsh, B. A., Congdon, J. D., Hinton, T. G., Whicker, F. W., & Bedford, J. S. (2000, in press). Culture methods for turtle lymphocytes. Methods in Cell Science.

Ulsh, B. A., Dugan, L., Hinton, T. G., Whicker, F. W., & Bedford, J. S. (2000, in press). Environmental biodosimetry: A biologically relevant tool for ecological risk assessment and biomonitoring. Journal of Environmental Radioactivity.

Ulsh, B. A., et. al. (2000, Jun.). Chromosome translocations in turtles: A biomarker in a sentinel animal for ecological dosimetry. Radiat. Res. 153(6), 752-759.

Ulsh, B. A., Whicker, F. W., Hinton, T. G., Congdon, J. D., & Bedford, J. S. (2000, in press). Chromosome translocations in T. scripta: The dose-rate effect and in vivo lymphocyte radiation response. Radiation Research.

Whicker, F. W. (2000). Radioecology: Relevance to problems of the new millennium. Journal of Environmental Radioactivity. 50, 173-178.

Publication Type: Poster

Bedford, J. S. (1998, Apr.). Development of a whole-chromosome painting probe for T. scripta. Radiation Research Society Annual Meeting, Louisville, KY.

Bedford, J. S. (1998, Dec.). Determining significant endpoints for ecological risk analyses. DOE/DoD/EPA Strategic Environmental Research and Development Program, Washington, D. C.

Bedford, J. S. (1998, Feb.). Non-mammalian whole chromosome FISH probes and microdissection. Third International Clinical FISH Symposium, Steamboat Springs, CO.

Bedford, J. S. (1998, Jul.). Determining significant endpoints for ecological risk analyses. DOE Environmental Management Science Program Workshop, Chicago, IL.

Bedford, J. S. (1999). Chromosome translocations in turtles: A biomarker for radiation exposure. International Congress on Radiation Research, Dublin, Ireland.

Bedford, J. S. (1999). Chromosome translocations in turtles: A biomarker for radiation exposure. Wildlife Applications in Remediation Decision Making Conference, Denver, CO.

Bedford, J. S. (1999, Apr.). Determining significant endpoints for ecological risk analyses. DOE Environmental Management Science Program Workshop, Atlanta, GA.

Bedford, J. S. (2000, Oct.). Chromosome translocations in turtles: A biomarker in a sentinel animal for environmental biodosimetry. International Workshop on Comparative Radiobiology, Dublin, Ireland.

Publication Type: Presentation

Bedford, J. S. (1999, Jul.). A chromosome runs through it. Invited speaker at the Thirty-Sixth Failla Award Lecture. Presented at the Eleventh International Congress of Radiation Research, Dublin, Ireland.

Hinton, T. G. (1999, Aug.). Determining significant endpoints for ecological risk analyses. Invited speaker at the DOE Biota Dose Assessment Group, Washington, D. C.

Hinton, T. G. (2000, Aug.). Determining significant endpoints for ecological risk analyses. Invited speaker at the International Atomic Energy Agency, Vienna, Austria.

Ulsh, B. A. (1999). Including reptiles and amphibians in ecological risk assessment. Invited speaker at the Wildlife Applications in Remediation Decision Making Conference, Denver, CO.

Ulsh, B. A. (2000, Nov.). Chromosome translocations in turtles: A biomarker in a sentinel animal for environmental biodosimetry. Society of Environmental Toxicology and Chemistry Annual Meeting, Nashville, TN.

Whicker, F. W. (1999, Jun.). Future directions in environmental and radiological research. Invited speaker at the 44th Annual Meeting of the Health Physics Society, Philadelphia, PA.

Whicker, F. W. (1999, May). Protection of the environment from ionizing radiation: An international perspective. Invited speaker at the 2nd International Symposium on Ionizing Radiation, Ottawa, Ontario, Canada.

Project: 59828

Title: Bioavailability of Organic Solvents in Soils: Input into Biologically Based Dose-Response Models for Human Risk Assessments

PI: Dr. Ronald C. Wester *Institution:* University of California at San Francisco

Publication Type: Journal

Poet, T. S., Corley, R. A , Thrall, K. D., & Wester, R. C. (1999). Assessing the dermal bioavailability of volatile organics in rats. The Toxicologist. 48, 339.

Poet, T. S., Corley, R. A., Thrall, K. D., Edwards, J. A., & Wester, R. C. (2000). Exhaled breath analysis and PBPK modeling of the dermal absorption of trichloroethylene in rats. The Toxicologist. 54, 147.

Poet, T. S., et. al. (2000, in press). Bioavailability of organic solvents in soils: Input into biologically based dose-response models for human-risk assessment. Proceedings of the 15th Annual International Conference on Contaminated Soils and Water.

Poet, T. S., et. al. (2000, Jul.). Assessment of the percutaneous adsorption of trichloroethylene in rats and humans using MS/MS real time breath analysis and physiological based pharmacokinetic modeling. Toxicol. Sci. 56(1), 61-72.

Poet,T. S., et. al. (2000, Mar.). Utility of real time breath analysis and physiologically based pharmacokinetic modeling to determine the percutaneous absorption of methyl chloroform in rats and humans. Toxicol. Sci. 54(1), 42-51.

Thrall, K., et. al. (2000). A real-time in vivo method for studying the percutaneous adsorption of volatile chemicals. Int. J. of Occupational and Environmental Health. 6, 96-103.

Wester, R. C., et. al. (1999). An innovative method to detemrine dermal uptake of solvents from soil and water in vivo in humans. The Toxicologist. 48, 338.

Wester, R. C., et. al. (2000). Human dermal absorption of trichloroethylene from soil and water. The Toxicologist. 54, 148.

Publication Type: Other

Thrall, K. D., Poet, T. S., & Corley, R. A. (1999). An innovative method to determine percutaneous absorption: Real time breath analysis and physiologically based pharmacokinetic modeling. Bronaugh, R. & Maibach, H. (Eds.), Percutaneous Absorption, Third Edition, Marcel Dekker, Inc. New York, NY.

Publication Type: Presentation

Wester, R. C. (1998). Chemical manufactures association workshop of research planning. Research Triangle Park, NC.

Wester, R. C. (1998, Sept.). Dermal bioavailability. Presetation at NIOSH. Morgantown, WV.

Wester, R. C. (1999). An innovative method to determine dermal uptake of solvents from soil and water in vivo in humans. Presentation at the 15th Annual International Conference on Contaminated Soils and Water. Amherst, MA.

Wester, R. C. (1999). An innovative method to determine dermal uptake of solvents from soil and water. Presentation at the Faculty and Student Undergraduate Research Education Conference, Argonne National Laboratory. Argonne, IL.

Project: 60037

Title: Estimation of Potential Population Level Effects of Contaminants on Wildlife
PI: Dr. James Loar *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Sample, B. E. & Arenal, C. A. (1999). Allometric models for interspecies extrapolation of wildlife toxicity data. Bull. Environ. Contam. Toxicol. 62, 653-663.

Publication Type: Poster

Mann, L. K., Sample, B. E., Arenal, C., Rose, K. A., & Suter, G. W. (2000, Apr. 24-27). Estimation of population-level effects on wildlife based on individual-level exposures: Influence of life-history strategies. Poster presentation at the Environmental Management Science Program National Workshop, Atlanta, GA.

Sample, B. E. & Arenal, C. (1998, Nov. 15-19). Allometric models for interspecies extrapolation of wildlife toxicity data: Expanding the database. Presentation at the 19th annual SETAC meeting in Charlotte, NC.

Sample, B. E., Arenal, C. A., & Mann, L. K. (1999). Determination of sensitivity of birds and mammals to environmental contamination. Poster presentation at the SETAC annual meeting.

Sample, B. E., Arenal, C., & Mann, L. (1999, Nov. 14-18). Determination of sensitivity of birds and mammals to environmental contaminants. Poster presentation at the 20th Annual SETAC Meeting, Philadelphia, PA.

Sample, B. E., Rose, K., & Suter, G. (1998, Dec. 1-3). Estimation of potential population-level effects of contaminants on wildlife. Poster presentation at Partners in EnvironmentalTechnology 98, SERDP Technical Symposium and Workshop, Crystal City, VA.

Sample, B. E., Rose, K., & Suter, G. (1998, Jul. 27-30). Estimation of potential population-level effects of contaminants on wildlife. Poster presentation at the 1st Annual Environmental Management Science Program National Workshop, Chicago, IL.

Publication Type: Presentation

Sample, B. E., Rose, K., & Suter, II, G. W. (1998, Jul. 27-30). Estimation of potential population-level effects of contaminants on wildlife. Presentation at the 1st annual meeting of the U. S. Department of Energy Environmental Management Science Program. Chicago, IL.

Sample, B. E., Rose, K., & Suter, II, G. W. (1998, Dec. 1-3). Estimation of potential population-level effects of contaminants on wildlife. Presentation at the Partners in Environmental Technology 98: SERDP Technical Symposium and Workshop. Crystal City, VA.

Sample, B. E., Rose, K., & Suter, II, G. W. (1999, Apr.). Estimation of potential population-level effects of contaminants on wildlife. Platform presentation at the NorCal SETAC meeting. Concord, CA.

Sample, B. E., Rose, K., Suter, II, G. W., & Arenal, C. (1998, Nov. 15-19). Wildlife toxicity data and ecological risk assessment: Problems and solutions. Platform presentation at the 19th annual SETAC meeting. Charlotte, NC.

Publication Type: Proceeding

Sample, B. E., Rose, K. A., & Suter II, G. W. (1998, Oct.). Estimation of population-level effects on wildlife based on individual-level exposures: Influence of life history strategies. Proceedings of Symposium on Environmental Contaminants and Terrestrial Vertebrates: Effects on Populations, Communities, and Ecosystems. College Park, MD. 18-21.

Project: 73942 (Renewal of Project No. 59918)

Title: Improved Radiation Dosimetry Risk Estimates to Facilitate Environmental Management of Plutonium Contaminated Sites

PI: Dr. Bobby R. Scott *Institution:* Lovelace Biomedical & Environmental Research Institute

Publication Type: Journal

Cheng, Y. -S., Zhou, Y., & Chen, B. T. (1999, Oct.). Particle deposition in a cast of human oral airways. Aerosol Sci. Tech. 31(4), 286-300.

Hoover, M. D., & Newton, G. J. (1998). Performance testing of continuous air monitors for alpha-emitting radionuclides. Radiat. Prot. Dosim. 79(1-4), 499-504.

Hoover, M. D., et. al. (1998). Characterization of enriched uranium dioxide particles from a uranium handling facility. Radiat. Prot. Dos. 79(1-4), 57-62.

Hoover, M. D., Mewhinney, C. J., & Newton, G. J. (1999). Modular glovebox connector and associated good practices for control of radioactive and chemically toxic materials. Health Phys. 76(1), 66-72.

Osovets, S. V. & Scott, B. R. (1998, Mar. 6). Nonmonotonous character of dose-response relationships. Viniti No. ¼, 645, B98 (in Russian).

Scott, B. R. & Fencl, A. (1999). Variability in PuO2 intake by inhalation: Implications for worker protection at the US Department of Energy. Radiat. Prot. Dosim. 83(3), 221-232.

Scott, B. R. (1999). Evaluating the risk of death via the Hematopoietic syndrome mode from prolonged exposure of nuclear workers to radiation delivered at very low raters. Health Physics. 74, 545-553.

Scott, B. R. (1999). Transformation of C3H 10T1/2 cells. Letter to Editor, J. Radiol. Prot. 19(2), 177-179.

Scott, B. R. (1999). Variability in PuO2 intake by inhalation: Implications for worker protection at the U.S. Department of Energy. Radiation Protection Dosimetry. 83(3), 221-232.

Scott, B. R., Lyzlov, A. F., & Osovets, S. V. (1998). Evaluating the risk of death via the hematopoietic syndrome mode for prolonged exposure of nuclear workers to radiation delivered at very low rates. Health Physics. 74 (5), 545-553.

Publication Type: Other

Glissmeyer, J. A., et. al. (1999). American national standard for sampling and monitoring releases of airborne radioactive substances from the stacks and ducts of nuclear facilities. ANSI/HPS N13.1-1999, Health Physics Society. McLean, VA.

Guilmette, R. A. & Scott, B. R. (1998.) Radiation toxicology. In Wexler, P. (Ed.), Encyclopedia of Toxicology. 3, 5-18. Academic Press. San Diego, CA.

Publication Type: Poster

Scott, B. R., Hoover, M. D., Neft, R. E., & Fencl, A. F. (1999, Aug. 22-26). Recommendations for improving the interim radionuclide soil action levels for the Rocky Flats Cleanup Agreement. Poster presentation at the 218th American Chemical Society National Meeting. New Orleans, LA.

Publication Type: Presentation

Cheng, Y. -S., Yeh, H. C., Smith, S. M., Cheng, K. H., & Swift, D. L. (1998, Sept. 14-18). Deposition of ultrafine particles in the nasal and tracheobronchial airways. 1998 International Aerosol Conference. Edinburgh, UK.

Hoover, M. D. (1998, Apr. 24). Workplace air sampling methods and good practices. Technical Workshop on Air Sampling: The Big Picture. Savannah River Chapter, Health Physics Society. Aiken, SC.

Hoover, M. D. (1998, Jul. 12). Statistical considerations for aerosol sampling, professional enrichment short course. 43rd Annual Meeting of the Health Physics Society. Minneapolis, MN.

Hoover, M. D. (1999, Jan. 24). Statistical considerations for aerosol sampling. Professional Enrichment Short Course. 32nd Midyear Meeting of the Health Physics Society. Albuquerque, NM.

Hoover, M. D., Newton, G. J., & Cox, F. M. (1998, Jul. 15). Flow measurements with rotameters and appropriate corrections. 43rd Annual Meeting of the Health Physics Society. Minneapolis, MN.

Hoover, M. D., Newton, G. J., & Cox, F. M. (1998, Feb. 7). Sampling radioactive aerosols. American Academy of Health Physics Short Course. 31st Midyear Meeting of the Health Physics Society. Mobile, AL.

Scott, B. R. (1998, Aug.). Improved radiation dosimetry/risk estimates to facilitate environmental management of plutonium contaminated sites. Presentation at the American Chemical Society. New Orleans, LA.

Scott, B. R., et. al. (1998, Jul. 27-30). Evaluating the intake via inhalation of plutonium oxides for the stochastic exposure paradigm. Poster 13 presented at the Environmental Management Science Program Workshop. Chicago, IL.

A particle size analyzer deployed at Fernald which is currently used to supplies airborne particulate concentration and size data at the waste pits, the soil dryer and at buildings being removed. [see Project #74050, renewal of #59882]

Smith, S. M., Cheng, Y. S., & Yeh, H. C. (1998, Sept. 14-18). Diffusional deposition of ultrafine particles in human tracheobronchial airways. 1998 International Aerosol Conference. Edinburgh, UK.

Zhang, Z., Wang, X., & Cheng, Y. -S. (1998, Sept. 14-18). Flow pattern and aerosol deposition in the human oral airway. 1998 International Aerosol Conference. Edinburgh, UK.

Publication Type: Proceeding

Glissmeyer, J. A., et. al. (1999). American national standard for sampling and monitoring releases of airborne radioactive substances from the stacks and ducts of nuclear facilities. ANSI/HPS N13.1-1999, Health Physics Society. McLean, VA.

Scott, B. R. (1998). Improved radiation dosimetry/risk estimates to facilitate environmental management of plutonium contaminated sites. In Environmental Management Science Program Workshop, U. S. Department of Energy Publication CONF-980736. Washington, D. C. 25-26.

Project: 74050 (Renewal of Project No. 59882)

Title: Measurement of Radon, Thoron, Isotopic Uranium and Thorium to Determine Occupational and Environmental Exposure at US DOE Fernald

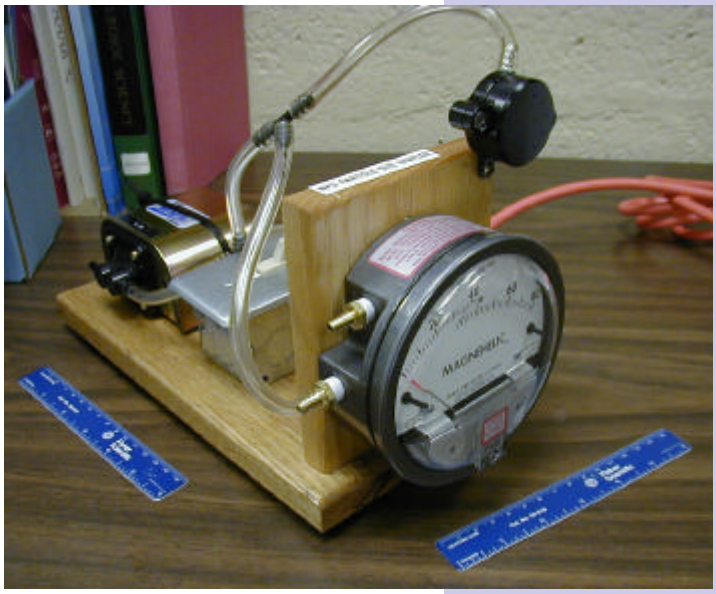
PI: Dr. Naomi H. Harley

Institution: New York University Medical School

Publication Type: Presentation

Harley, N. H. (1999, Jun.). Field results of personal radon and thoron monitor. Annual Health Physics Meeting. Philadelphia, PA. Health Physics. 76, 163.

Harley, N. H. (1999, Jun.). Results of particle size sampler field tests. Annual Health Physics Meeting. Philadelphia, PA. Health Physics. 76, 163.



A particle size analyzer that is used for size distribution measurements of inhaled radionuclides particles. Particle size is the major determinant of bronchial doses of radionuclides. [see Project #74050, renewal of #59882]

Low Dose Radiation

Project: 69904

Title: Low-Dose Risk, Decisions, and Risk Communication

PI: Dr. James Flynn

Institution: Decision Science Research Institute

Publication Type: Poster

Flynn, J. (2001, Jun.). Low dose risk, decision, & risk communication. U. S. Department of Energy/National Aeronautics and Space Administration. Washington, D. C.

Flynn, J. (2000, Apr.). The social geography of risk communication. U. S. Department of Energy, Environmental Management. Atlanta, GA.

Publication Type: Presentation

Flynn, J. (2001, Jun.). Low dose risk, decision, and risk communication. U. S. Department of Energy/National Aeronautics and Space Administration Radiation Investigator's Workshop. Hilton Arlington and Towers. Washington, D. C.

Flynn, J. (2001, Sept.). Public interaction and acceptance aspects. National Research Council, Board on Radioactive Waste Management, Workshop on Principles and Operational Strategies for Repository Siting Systems. Washington, D. C.

Flynn, J. (1999, Dec.). The role of risk communication in response to technological stigma. Society for Risk Analysis. Atlanta, GA.

Flynn, J. (1999, Nov.). The role of stigmatization in public risk perceptions of high-level radioactive wastes. Board on Radioactive Waste Management, National Research Council. Irvine, CA.

Flynn, J. (2000, Jan.). The social context for risk communication. National Cancer Institute/Center for Disease Control. Workshop on I-131 fallout from Nevada Test Site. Rockville, MD.

Flynn, J. (2000, Jul.). Radiation risk, decisions, and risk communication. Gordon Conference. Sawyer-Colby College. New London, CN.

Flynn, J. (2000, Jun.). Trust and risk management communications. International Conference on Trust. Western Washington State University. Bellingham, WA.

Flynn, J. (2001, Apr.). The social context for communication about radiation risk. American Chemical Society Symposium on Radiation Health and Safety: Myth and Reality. 221st ACS National Meeting. San Diego, CA.

Flynn, J. (2001, Mar.). The confusion of risk perception. DOE Workshop on the Communication of the Low-Dose Radiation Research Program. Freedom Forum World Center. Arlington, VA.

Project: 69939

Title: Sensitivity to Radiation-Induced Cancer in Hemochromatosis

PI: Dr. James E. Morris *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Stevens, R. G., Morris, J. E., & Anderson, L. E. (2000). Commentary: Hemochromatosis heterozygotes constitute a radiation-sensitive subpopulation. Rad. Res. 153, 844-847.

Publication Type: Presentation

Morris, J. E., Anderson, L. E., & Sasser, L. B. (2000, Sept.). Sensitivity to radiation-induced cancer in hemachromatosis. Conference on Radiation Protection for our National Priorities. Columbia Chapter. Health Physics Society. Spokane, WA.

HIGH-LEVEL WASTE

Actinide (Heavy Element) Chemistry

Project: 59977

Title: Synthesis and Characterization of Templated Ion Exchange Resins for the Selective Complexation of Actinide Ions

PI: Dr. George M. Murray *Institution:* Johns Hopkins University Applied Physics Lab

Publication Type: Journal

Bae, S. Y., Southard, G. L., & Murray, G. M., (1999 Oct. 4). Molecularly imprinted ion exchange resin for purification, preconcentration, and determination of UO22+ by spectrophotometry and plasma spectrometry. Anal. Chim. Acta. 397(1-3), 173-181.

Publication Type: Paper

Arnold, B. R., Jenkins, A. L., Uy, O. M., & Murray, G. M. (1999). Progress in the development of molecularly imprinted polymer sensors. JHUAPL Technical Digest. 20, 190-198.

Publication Type: Presentation

Kimaro, A. & Murray, G. M. (1998, Mar. 7-12). Synthesis and characterization of templated ion exchange resins for the selective complexation of actinide ions. Abstract No. 2315P, Pittsburgh Conference. Orlando, FL.

Project: 65370

Title: Actinide-Specific Interfacial Chemistry of Monolayer Coated Mesoporous Ceramics

PI: Dr. Glen E. Fryxell *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Feng, X., et. al. (1999). Self-assembled monolayers on mesoporous silica, a super sponge for actinides. In Mara, J. C. & Chandler, G. T. (Eds.), Ceramic Transactions, 93, Environmental Issues and Waste Management Technologies IV. 35-42.

Fryxell, G. E., et. al. (1999, Aug.). Design and synthesis of selective mesoporous anion traps. Chem. Mater. 11(8), 2148-2154.

Fryxell, G. E., Liu, J., & Mattigod, S. V. (1999, Dec.). Self-assembled monolayers on mesoporous supports (SAMMS) - an innovative environmental sorbent. Mater. Technol. 14(4), 188-191.

Publication Type: Other

Fryxell, G. E. & Liu, J. (1999, in press). Designing surface chemistry in mesoporous silica. In Papirer, E. (Ed.), Adsorption at Silica Surfaces. Marcel Dekker.

Publication Type: Presentation

Fryxell, G. E., et al. (1999, Jun.). Self-assembled monolayers on mesoporous supports: Synthesis of nanoscale hybrid materials and their applications. Presentation at the Northwestern Regional Meeting of the American Ceramic Society. Portland, OR.

Fryxell, G. E., et. al. (1999, Apr.). Design and synthesis of mesoporous lanthanide sorbent materials. Invited presentation at the 101st National Meeting of the American Ceramic Society.

Fryxell, G. E., et. al. (1999, Apr.). Environmental applications of interfacially modified mesoporous ceramics. Invited presentation at the 101st National Meeting of the American Ceramic Society.

Fryxell, G. E., et. al. (1999, Aug.). Environmental applications of Self-Assembled Monolayers on Mesoporous Supports (SAMMS). Invited presentation at the National Meeting of the American Ceramic Society. New Orleans, LA.

Fryxell, G. E., et. al. (1999, Jun.). High efficiency environmental sorbent materials: Self-assembled Monolayers on Mesoporous Support (SAMMS) for metal removal from aqueous systems. Presentation at the Symposium on Environmental Chemistry at the Northwestern Regional Meeting of the American Chemical Society. Portland, OR.

Fryxell, G. E., et. al. (1999, Jun.). High efficiency environmental sorbent materials: Self-assembled Monolayers on Mesoporous Supports (SAMMS) for metal removal from aqueous systems. Presentation at the Northwestern Regional Meeting of the American Ceramic Society. Portland, OR.

Fryxell, G. E., et. al. (1999, Jun.). Self assembled monolayers on mesoporour supports: Synthesis of nanoscale hybrid materials and their applications. Presentation at the Symposium on Nanoscale Materials at the Northwestern Regional Meeting of the American Chemical Society. Portland, OR.

Fryxell, G. E., Zemanian, T. S., & Yin, Y. H. (1999, Aug. 22). Environmental applications of self-assembled monolayers on mesoporous supports. Abstr. Pap. Am. Chem. S. 218, U1089-U1089, Part 1.

Publication Type: Press release

Fryxell, G. E. (1999, Apr. 11). PNNL focuses on healthy environment. Tri-City Herald, D1.

Fryxell, G. E. (1999, Mar.). Metal eaters. Popular Science, 34.

Project: 73749 (Renewal of Project No. 54621)

Title: Chemical Speciation of Strontium, Americium, and Curium in High Level Waste: Predictive Modeling of Phase Partitioning During Tank Processing

PI: Dr. Andrew R. Felmy *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Felmy, A. R. & Mason, M. J. (1998). The displacement of strontium from organic chelates by hydroxide, carbonate, and calcium in concentrated electrolytes. Journal of Solution Chemistry. 27(5), 435-454.

Felmy, A. R. & Rai, D. (1999, May). Application of Pitzer's equations for modeling the aqueous thermodynamics of actinide species in natural waters: A review. J. Solution Chem. 28(5), 533-553.

Felmy, A. R., Dixon, D. A., Rustad, J. R., Mason, M. J. & Onishi, L. M. (1998). The hydrolysis and carbonate complexation of strontium and calcium in aqueous electrolytes: Use of molecular modeling calculations in the development of aqueous thermodynamic models. J. Chem. Thermodyn. 30, 1103-1120.

Oakes, C. S., Sterner, S. M. & Felmy, A. R. (2000, Jan.). Thermodynamic properties of aqueous calcium nitrate [Ca(NO3)(2)] to the temperature 373K including new enthalpy of dilution data. J. Chem. Thermodyn. 32(1), 29-54.

Sterner, S. M., Felmy, A. R., Oakes, C. S., & Pitzer, K. S. (1998). Correlation of thermodynamic data for aqueous electrolyte solutions to very high ionic strength using INSIGHT: Vapor saturated water activity in the system CaCl2-H2O to 250 ° C and solid saturation. International Journal of Thermophysics. 193, 761-770.

Publication Type: Presentation

Felmy, A. R., Choppin, G. R., Dixon, D. A., & Campbell, J. A. (1998, Jul. 27-30). Chemical speciation of strontium, americium, and curium in high-level waste: Predictive modeling of phase partitioning during tank processing. Two presentations and one poster. Presentations to the Hanford Tanks Site Technology Coordination Group (STCG) on November 10, 1998, and to PNNL staff on January 21, 1998. Poster presentation at the EMSP Principal Investigators Workshop, Chicago, IL.

Felmy, A. R. & Mason, M. J. (1998, Aug. 9-14). The aqueous complexation of Eu(III) with organic chelating agents at high base and high ionic strengths: Metal-chelate displacement induced by hydrolysis and precipitation reactions. 53rd Calorimetry Conference. Midland, MI.

Felmy, A. R., Dixon, D. A. & Mason, M. J. (1997, Aug. 3-8). The complexation of alkaline earth cations by organic chelates at high ionic strength: Competitive effects of hydrolysis and carbonate complextion. 52nd Calorimetry Conference. Asilomar, CA.

Felmy, A. R., Dixon, D. A. & Mason, M. J. (1999, Mar. 21-25). Aqueous complexation of Eu(III) with organic chelating agents at high base concentration: Molecular and thermodynamic modeling results. 217th ACS National Meeting. Anaheim CA.

Felmy, A. R., Dixon, D. A., Campbell, J. A. & Mason, M. J. (1997, Sept. 7-11). The effects of OH, CO3, and Ca on the displacement of strontium from organic chelates: Implications for waste processing. 214th ACS National Meeting. Las Vegas, NV.

Felmy, A. R., Dixon, D. A., Rustad, J. R., Mason, M. J. & Onishi, L. M. (1997, Aug. 3-8). The use of molecular modeling calculations to improve the development of thermodynamic models: Hydrolysis, carbonate, and EDTA complexation of alkaline earth cations. 52nd Calorimetry Conference. Asilomar, CA.

Oakes, C. S. & Felmy, A. R. (1997, Aug. 3-8). Thermodynamics of [Na4EDTA+NaOH]{aq}, including new isopiestic measurements, to 373K, 0.1MPa, and stoichiometric ionic strengths of 18 . 9mol . kg -1. 52nd Calorimetry Conference, Asilomar, CA.

Oakes, C. S. & Felmy, A. R. (1998, Aug. 9-14). Thermodynamics of [Na4EDTA+NaOH]{aq}, including new isopiestic and enthalpy of dilution measurements. 53rd Calorimetry Conference. Midland, MI.

Petersen, C. E., Campbell, J. A., Felmy, A. R., Wahl, K. L. & Finch, J. W. (1998, May 31-June 4). Analysis of metal-organic complexes using CE/MS. 46th American Society of Mass Spectrometry Meeting. Orlando, FL.

Sterner, S. M., Felmy, A. R. & Pitzer, K. S. (1997, Jun. 22-27). Correlation of thermodynamic data for aqueous electrolyte solutions to very high ionic strength using INSIGHT: Vapor saturated water activity in the system CaCl2-H2O to 250 ° C and solid saturation. Thirteenth Symposium on Thermophysical Properties. Boulder, CO.

Sterner, S. M., Felmy, A. R., Oakes, C. S., Simonson, J. M., & Pitzer, K. (1997, Aug. 3-8). Thermodynamics of aqueous CaCl2 to 250 ° C, 400 bars and solid saturation. 52nd Calorimetry Conference. Asilomar, CA.

Publication Type: Report

Boger, M. (2001). Results of the MVDSS radiological screening activity were released as a supporting document. RPP-7522, Rev. 0. NHC (376-3355).

Vienna, J. (2001). A PNNL letter report describing the status of studies on the impact of crystallinity on the PCT response of HLW glasses was issued. PNNL (372-2807).

Boger, M. (2001). Mobile variable depth sampling system conceptual design review report. RPP-8147, Rev. 0. NHC (376-3355).

Project: 73759 (Renewal of Project No. 54679)

Title: Computational Design of Metal Ion Sequestering Agents

PI: Dr. Benjamin P. Hay *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Bryan, J. C., Delmau, L. H., & Hay, B. P. (1999, Jun.). Cesium recognition by supramolecular assemblies of 2-benzylphenol and 2-benzylphenolate. Struct. Chem. 10(3), 187-203.

Bryan, J. C., Sachleben, R. A., & Hay, B. P. (1999, Jun. 30). Structural aspects of cesium ion selectivity by tetrabenzo-24-crown-8. Inorg. Chim. Acta. 290(1), 86-94.

Clement, O., Rapko, B. M., & Hay, B. P. (1998). Structural aspects of metal-amide complexes. Coordination Chemistry Reviews. 170, 203.

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Hay, B. P., Clement, O., & Sandrone, G. (1998, Nov. 2). A molecular mechanics (MM3(96)) force field for metal-amide complexes. Inorg. Chem. 37(22), 5887-5894.

Hay, B. P., Clement, O., Sandrone, G., & Dixon, D. A. (1998). A MM3(96) force field for metal amide complexes. Inorganic Chemistry. 37, 5887.

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McNamara, B. K., Lumetta, G. J. & Rapko, B. M. (1999). Extraction of europium(III) ion with tetrahexylmalonamides. Solvent Extr. Ion. Exc. 17(6), 1403-1421.

Rao, L., Xia, Y., Rapko, B. M., & Martin, P. F. (1998). Synergistic extraction of Eu(III) and Am(III) by thenoyltrifluoroacetone and neutral donor extractants: Octyl(phenyl)-N,N-diisobutylcarbonyl-methylphosphine oxide and 2,6-bis(diphenylphosphino)methyl pyridine N,P,P trioxide. Solvent Extraction and Ion Exchange. 16, 913.

Rapko, B. M., McNamara, B. K., Lumetta, G. J., Rogers, R. D., & Hay, B. P. (1999, Oct. 4). Ordination of lanthanide nitrates with N,N,N,'N'-tetramethylsuccinamide. Inorg. Chem. 38(20), 4585-4592.

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Publication Type: Other

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Publication Type: Presentation

Clement, O., Hay, B. P. Dixon, D. A., & Sandrone, G. (1998, Jun.). A MM3(96) force field for metal-amide complexes. West Coast Theoretical Chemistry Conference. Richland, WA.

Clement, O., Sandrone, G., Dixon, D. A., & Hay, B. P. (1998, Mar.). A MM3(96) force field for metal-amide complexes. 215th American Chemical Society National Meeting, Dallas, TX.

Clement, O., Sandrone, G., Dixon, D. A., & Hay, B. P. (1998, Jun.). A MM3(96) force field for metal-amide complexes. 53rd Northwest Regional American Chemical Society Meeting. Pasco, WA.

Hay, B. P. (1998, Aug.). A points-on-a-sphere approach to model metal-ligand interactions with an extended MM3 model. Invited presentation at the 216th American Chemical Society National Meeting, Boston, MA.

Hay, B. P. (1998, Jul.) Architectural design criteria for f-block metal sequestering agents. Environmental Management Science Program Workshop. Chicago, IL.

Hay, B. P. (1998, Oct.). Ligand design with molecular mechanics. INEEL Science Integrated Workshop, Environmental Management Science Program. Idaho Falls, ID.

Hay, B. P. (1999, Jun.) The application of molecular mechanics in the design of metal ion sequestering agents. Invited presentation at the Metal Separation Technologies Beyond 2000: Integrating Novel Chemistry with Processing United Engineering Foundation Conference. Turtle Bay, Oahu, HI.

Hay, B. P., Dixon, D. A., & Sandrone, G. (1998, Jun.). A modified MM3(96) force field for simple amides and diamides. West Coast Theoretical Chemistry Conference. Richland, WA.

Hay, B. P., Dixon, D. A., & Sandrone, G. (1998, Jun.). A modified MM3(96) force field for simple amides and diamides. 53rd Northwest Regional American Chemical Society Meeting. Pasco, WA.

Lumetta, G. J., McNamara, B. K., & Burgeson, E. (1997, Jun). Amide complexes of f-block elements. 21st Annual Actinide Separations Conference. Charleston, SC.

Lumetta, G. J., McNamara, B. K., & Rapko, B. M. (1998, Jun.). Binding of diamide ligands to f-block elements. 53rd Northwest Regional American Chemical Society Meeting. Pasco, WA.

Lumetta, G. J., McNamara, B. K., & Rapko, B. M. (1998, Apr.). Binding of amide ligands to f-block elements. 22nd Annual Actinide Separations Conference. Chattanooga, TN.

Lumetta, G. J., McNamara, B. K., & Rapko, B. M. (1999, Mar.). Equilibrium modeling of the extraction of f-block elements by diamides. 217th American Chemical Society National Meeting. Anaheim, CA.

Rao, L., Zanonato, P., & Di Bernardo, P. (1998, Aug.). Thermodynamics of europium(III) complexation with alkyl-substituted diamides in organic solvents. 216th American Chemical Society National Meeting. Boston, MA.

Rapko, B. M. (1997, Apr.) Extraction of f-elements by phosphine oxide/pyridine N-oxide ligands. 213th American Chemical Society National Meeting. San Francisco, CA.

Rapko, B. M., et al. (1999, Mar.). Coordination chemistry of tetraalkyldiamides with f-block metal salts. 217th American Chemical Society National Meeting. Anaheim, CA.

Rapko, B. M., et. al. (1999, Jun.). Coordination chemistry of diamides with f-block metal salts. Metal Separation Technologies Beyond 2000: Integrating Novel Chemistry with Processing United Engineering Foundation Conference. Turtle Bay, Oahu, HI.

Rapko, B. M., Lumetta, G. J., McNamara, B. K., Rao, L., & Zanonato, P. L. (1997, Oct.). Determination of actinide and lanthanide binding constants with amides and diamides. Tenth Symposium on Separation Science and Technology for Energy Applications. Gatlinburg, TN.

Rapko, B. M., McNamara, B. K., Rogers, R. D., Lumetta, G. J., & Hay, B. P. (1998, Jun.). Coordination chemistry of lanthanide salts with N,N,N',N'-tetramethylsuccinamide and N,N,N',N'-tetrahexyl-succinamide. 53rd Northwest Regional American Chemical Society Meeting. Pasco, WA.

Roundhill, D. M. (1998, May). New macrocycles for selective ion exchange. Metals Adsorption Workshop. Cincinnati, OH.

Roundhill, D. M. (1999, Mar.). Calixarene amines and amides as extractants for oxyions. 217th National American Chemical Society National Meeting. Anaheim, CA.

Yordanov, A. T., Wolf, N. J., Koch, H. F., & Roundhill, D. M. (1998, Jun.). Sulfur and nitrogen derivatized calix[4]arenes as selective phase transfer extractants for heavy metals and oxyions. Second Fargo Conference on Main Group Chemistry. Fargo, ND.

Zanonato, P. L. & Rao, L. (1997, Sept.). Complexation of Eu(III) by N,N,N',N'-tetra-alkyldiamides. 214th American Chemical Society National Meeting. Las Vegas, NV.

Publication Type: Proceeding

Hay, B. P. (1999, in press). The use of molecular mechanics in the design of metal ion sequestering agents. In Metal separation technologies beyond 2000: Integrating novel chemistry with processing. United Engineering Foundation. New York, NY.

Hay, B. P., Dixon, D. A., Lumetta, G. J., & Rapko, B. M. (1998). Environmental management science program workshop. CONF-980736, Environmental Management Science Program, U.S. Department of Energy, Office of Science and Risk Policy EM-52. Washington, D.C.

Rao, L., Xia, Y., Rapko, B. M., & Martin, P. L. (1997, Jun). Synergistic extraction of Eu(III) and Am(III) by TTA and the neutral donor extractants CMPO and NOPOPO. 21st Annual Actinide Separations Conference. Charleston, SC.

Publication Type: Report

Hay, B. P., Dixon, D. A., Lumetta, G. J., & Rapko, B. M. (1997). Science to Support DOE Site Cleanup: The Pacific Northwest National Laboratory Environmental Management Science Program Awards. Fiscal Year 1997 Mid-Year Progress Report. PNNL-11589, Pacific Northwest National Laboratory. Richland, WA.

Hay, B. P., Dixon, D. A., Lumetta, G. J., & Rapko, B. M. (1998). Science to Support DOE Site Cleanup: The Pacific Northwest National Laboratory Environmental Management Science Program Awards. Fiscal Year 1998 Mid-Year Progress Report. PNNL-11899, Pacific Northwest National Laboratory. Richland, WA.

Lumetta, G. J., Rapko, B. M., & McNamara, B. K. (1999). The SX solver: A new computer program for analyzing solvent extraction equilibria. PNNL-12085, Pacific Northwest National Laboratory. Richland, WA.

Project: 81887 (Renewal of Project No. 65411)

Title: Precipitation and Deposition of Aluminum-Containing Phases on Tank Wastes

PI: Dr. Shas Mattigod *Institution:* Pacific Northwest National Laboratory

Publication Type: Proceeding

Liu, J., et. al. (1999, Aug. 22). Characterization of colloidal phases in tank wastes. Abstr. Pap. Am. Chem. S. 218, U1077-U1077, Part 1.

Project: 81896

Title: Speciation, Dissolution, and Redox Reactions of Chromium Relevant to Pretreatment and Separation of High-level Tank Wastes

PI: Dr. Dhanpat Rai *Institution:* Pacific Northwest National Laboratory

Publication Type: Poster

Rai, D., Rao, L., Clark, S. B., Hess, N. J., & Felmy, A. R. (2000). Speciation, dissolution, and redox reactions of chromium relevant to pretreatment and separation of high-level tank wastes. EMSP National Workshop. Atlanta, GA.

Publication Type: Presentation

Friese, J., et. al. (2000, Mar.). Oxidation of trivalent Cr using oxidants relevant to high-level radioactive waste. 219th American Chemical Society National Meeting. San Francisco, CA.

Friese, J., Ritherdon, B., Clark, S. B., Rao, L., & Zhang, Z. (2001, Apr.). Removing chromium from high-level radioactive waste streams: Speciation and reactivity of Cr(III) oligometers under highly alkaline conditions. 221st American Chemical Society National Meeting. San Diego, CA.

Rai, D., Rao, L., Clark, S. B., Hess, N. J., & Felmy, A. R. (2000, Mar.). Solubility of Cr(III) compounds and their redox transformation reactions: Application to pretreatment of high-level waste sludges. EMSP National Workshop. Atlanta, GA.

Rao, L., et. al. (1999, Aug.). Speciation, dissolution, and redox reactions of Cr(III) in alkaline solutions. 218th American Chemical Society National Meeting. New Orleans, LA.

Rao, L., et. al. (2000, Mar.). Dissolution of Cr(OH)3(am)/Cr2O3(c) and oxidation of Cr(III) in alkaline solutions. 219th American Chemical Society National Meeting. San Francisco, CA.

Publication Type: Report

Rai, D., Rao, L., Clark, S. B., Hess, N. J., & Lumetta, G. J. (2000). Speciation, dissolution, and redox reactions of chromium relevant to pretreatment and separation of high-level tank wastes. In Science to Support DOE Site Cleanup: The Pacific Northwest National Laboratory Science Program Awards. PNNL-12208. Pacific Northwest National Laboratory. Richland, WA. 1.15-1.17.

Rai, D., Rao, L., Clark, S. B., Hess, N. J., & Lumetta, G. J. (1999). Speciation, dissolution, and redox reactions of chromium relevant to pretreatment and separation of high-level tank wastes. In Science to Support DOE Site Cleanup: The Pacific Northwest National Laboratory Science Program Awards. PNNL-12208. Pacific Northwest National Laboratory. Richland, WA. 1.61-1.86.

Project: 81962 (Renewal of Project No. 65352)

Title: Understanding the Chemistry of the Actinides in High Level Waste Tank Systems: The Impact of Temperature on Hydrolysis and Complexation with Organics

PI: Dr. Sue B. Clark *Institution:* Washington State University

Publication Type: Journal

Clark, S. B. (1999, in press). The aqueous geochemistry of the rare earth elements. IX. A potentiometric study of Nd 3+ complexation with acetate in 0.1 molal NaCl solutions from 25-225° C. Geochim. Cosmochim. Acta.

Yeh, M., Maddison, A., & Clark, S. B. (2000, Mar.). Temperature dependence of chloride complexation for the trivalent f-elements. J. Radioanal. Nucl. Ch. 243(3), 645-650.

Yeh, M., Riedener, T., Bray, K., & Clark, S. B. (2000, May 24). A spectroscopic investigation of temperature effects on solution complexation in the Eu 3+ -acetate system. Journal of Alloys and Compounds.

Publication Type: Paper

Wood, S. A., Palmer, D. A., Wesolowski, D. J. (1999, Aug. 22-27). Determination of the solubility of crystalline Nd(OH)3 in sodium triflate solutions from 30 to 250 C with in situ pH measurement. Determination of the solubility of crystalline Nd(OH)3 in sodium triflate solutions from 30 to 250 C with in situ pH measurement. Ninth Annual V.M. Goldschmidt Conference Abstracts. Harvard University, Cambridge, MA. Lunar and Planetary Institute Contribution No. 791. Houston, TX. 329-330.

Analytical Chemistry & Instrumentation

Project: 55318

Title: Improved Analytical Characterization of Solid Waste Forms by Fundamental Development of Laser Ablation Technology

PI: Dr. Richard E. Russo *Institution:* Lawrence Berkeley National Laboratory

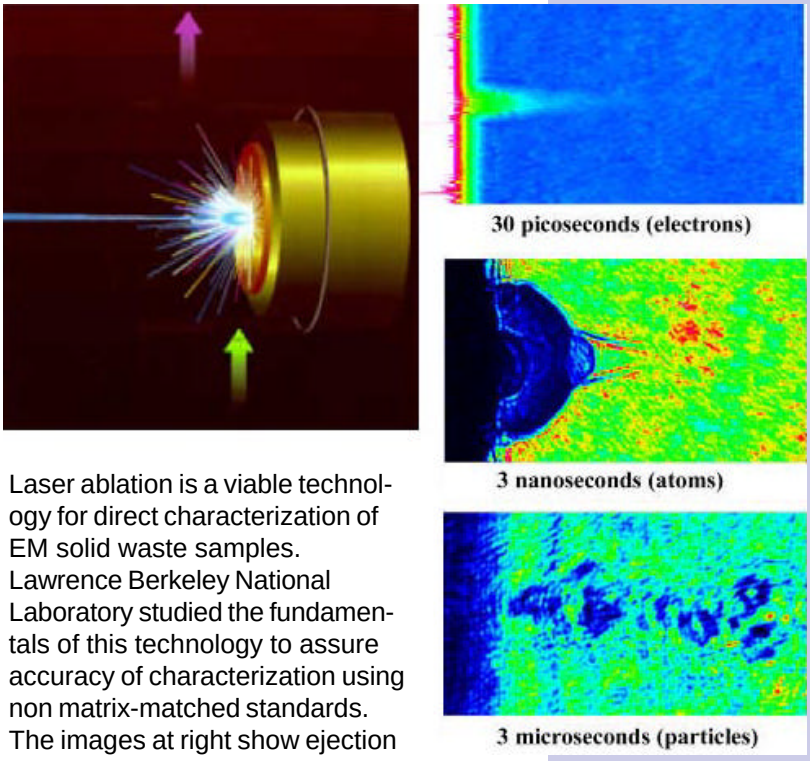
Publication Type: Journal

Borisov, O. V., Mao, X. L., & Russo, R. E. (1999, in press). Laser ablation ICP/MS calibration based on binary Cu/Zn alloy standards. Spectrochimica Acta B.

Borisov, O. V., Mao, X. L., Ciocan, A. C., & Russo, R. E. (1998). Time resolved parametric studies of laser ablation using ICP-AES. Applied Surface Science. 129, 315.

Chan, W. T., Leung, A. P. K., Mao, X. L., & Russo, R. E. (1998). Effects of gas environment on pico-second laser ablation. Applied Surface Science. 129, 269.

Ciocan, A. C., Mao, X. L., Borisov, O. V., & Russo, R. E. (1998). Optical emission spectroscopy of the influence of laser ablated mass on dry inductively coupled plasma conditions. Spectrochimica Acta. 53B, 463.



Laser ablation is a viable technology for direct characterization of EM solid waste samples. Lawrence Berkeley National Laboratory studied the fundamentals of this technology to assure accuracy of characterization using non matrix-matched standards. The images at right show ejection of electrons, atoms, and particles at different times during an ablation event. Understanding the contribution of each mass form to the chemical analysis is one of the goals of this research. [see Project #55318]

Jeong, S. H., Borisov, O. V., Yoo, J. H., Mao, X. L., & Russo, R. E. (1999, Nov. 15). Effects of particle size distribution on inductively coupled plasma mass spectrometry signal intensity during laser ablation of glass samples. Anal. Chem. 71(22), 5123-5130.

Leung, A. P. K., Chan, W. T., Mao, X. L., & Russo, R. E. (1998). Influence of gas atmosphere on picosecond laser ablation sampling efficiency and ICP-AES. Analytical Chemistry. 70(N22), 4709.

Liu, H. C., et. al. (1999, Nov. 8). Early phase laser induced plasma diagnostics and mass removal during single-pulse laser ablation of silicon. Spectrochim. Acta. B. 54(11), 1607-1624.

Russo, R. E. (1998). Laser ablation sampling. Trends in Analytical Chemistry (Personal Edition). 17(8-9).

Russo, R. E. (1998, Jul. 1). Transient isotachophoretic - electrophoretic separations of lanthanides with indirect laser-induced fluorescence detection. Analytical Chemistry. 70(13).

Russo, R. E. (1998, Jul. 18). Preferential vaporization during laser ablation inductively coupled plasma atomic emission spectroscopy. Applied Spectroscopy. 52(7).

Russo, R. E. (1998, Mar. 30). Optical emission spectroscopy studies of the influence of laser ablated mass on dry inductively coupled plasma conditions. Spectrochimica Acta, Part B: Atomic Spectroscopy. 53(3).

Russo, R. E. (1998, May 29). Enhancements in laser ablation inductively coupled plasma-atomic emission spectrometry based on laser properties and ambient environment. Spectrochimica Acta, Part B: Atomic Spectroscopy. 53(5).

Publication Type: Presentation

Borisov, O. V., Mao, X. L., & Russo, R. E. (1998, Oct.). Optimization of ICPMS for laser ablation sampling. 25th Annual Conference of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS). Austin, TX.

Chan, W. -T., Leung, A. P. K., Mao, X. L., & Russo, R. E. (1997, Oct.). Effect of gas medium on laser ablation sampling for ICP-AES. Twenty-Fourth Annual Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies. (FACSS). Providence, RI.

Chan, W. T., Leung, A. P. K., Mao, X. L., & Russo, R. E. (1997, Jul.). Effects of gas atmosphere on pico-second laser ablation sampling for ICP-AES. Fourth International Conference on Laser Ablation (COLA 97). Asilomar, CA.

Ciocan, A. C., Mao, X. L., Borisov, O. V., & Russo, R. E. (1997, Jul.). Optical emission spectroscopy of the influence of ablated material on dry inductively coupled plasma conditions. COLA 97. Asilomar, CA.

Russo, R. E. (1998, Sept.). Laser-ablation sampling with ICP/AES and ICP/MS: Fundamental issues to improve analytical applications. Invited presentation at the Society of Applied Spectroscopy California Section Meeting. Fremont, CA.

Russo, R. E. (1999, Apr.). Fundamental and applied aspects of laser ablation for chemical analysis. Frontiers in Chemistry Lecture Series. Wayne State University. Detroit, MI.

Russo, R. E., Jeong, S. H., Mao, X. L., Borisov, O. V., & Yoo, J. (1998, Oct.). Particle generation and transport during laser ablation sampling for chemical analysis. 25th Annual Conference of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS). Austin, TX.

Russo, R. E., Mao, X. L., Ciocan, A. C., & Borisov, B. V. (1997, Oct.). Laser ablation solid sample chemical analysis: Dream or reality. Invited presentation at the Twenty-Fourth Annual Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS). Providence, RI.

Russo, R. E., Mao, X. L., Ciocan, A. C., & Borisov, B. V. (1997, Oct.). Laser ablated mass influence on the properties of the ICP. Invited presentation at the Twenty-Fourth Annual Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies. (FACSS). Providence, RI.

Publication Type: Proceeding

Borisov, O. V., Mao, X. L. & Russo, R. E. (1999, Apr.). Direct characterization of solid waste forms using laser ablation ICPMS. Waste Management Science and Technology in the Ceramic and Nuclear Industries. American Ceramic Society.

Chan, W. T., Leung, A. P. K., Mao, X. L., & Russo, R. E. (1997). Effects of gas atmosphere on pico-second laser ablation sampling for ICP-AES. Fourth International Conference on Laser Ablation (COLA 97). Asilomar, CA.

Ciocan, A. C., Mao, X. L., Borisov, O. V., & Russo, R. E. (1997, Jul.). Optical emission spectroscopy studies of ablated material on dry inductively coupled plasma conditions. COLA. Asilomar, CA.

Mao, X. L., Ciocan, A. C., Borisov, O. V., & Russo, R. E. (1997, Jul.). Time resolved parametric studies of laser ablation of brass using ICP-AES. COLA 97. Asilomar, CA.

Russo, R. E. (1997, Jul. 21-25). Effects of gas environment on picosecond laser ablation. Applied Surface Science Proceedings of the 1997 4th International Conference on Laser Ablation.

Russo, R. E. (1997, Jul. 21-25). Propagation of the shock wave generated from excimer laser heating of aluminum targets in comparison with ideal blast wave theory. Applied Surface Science Proceedings of the 1997 4th International Conference on Laser Ablation.

Russo, R. E. (1997, Jul. 21-25). Time-resolved parametric studies of laser ablation using inductively coupled plasma atomic emission sectroscopy. Applied Surface Science Proceedings of the 1997 4th International Conference on Laser Ablation.

Russo, R. E., Mao, X. L., & Borisov, O. V. (1998). Laser Ablation Sampling. Trends in Analytical Chemistry. 17, 461.

Project: 59978

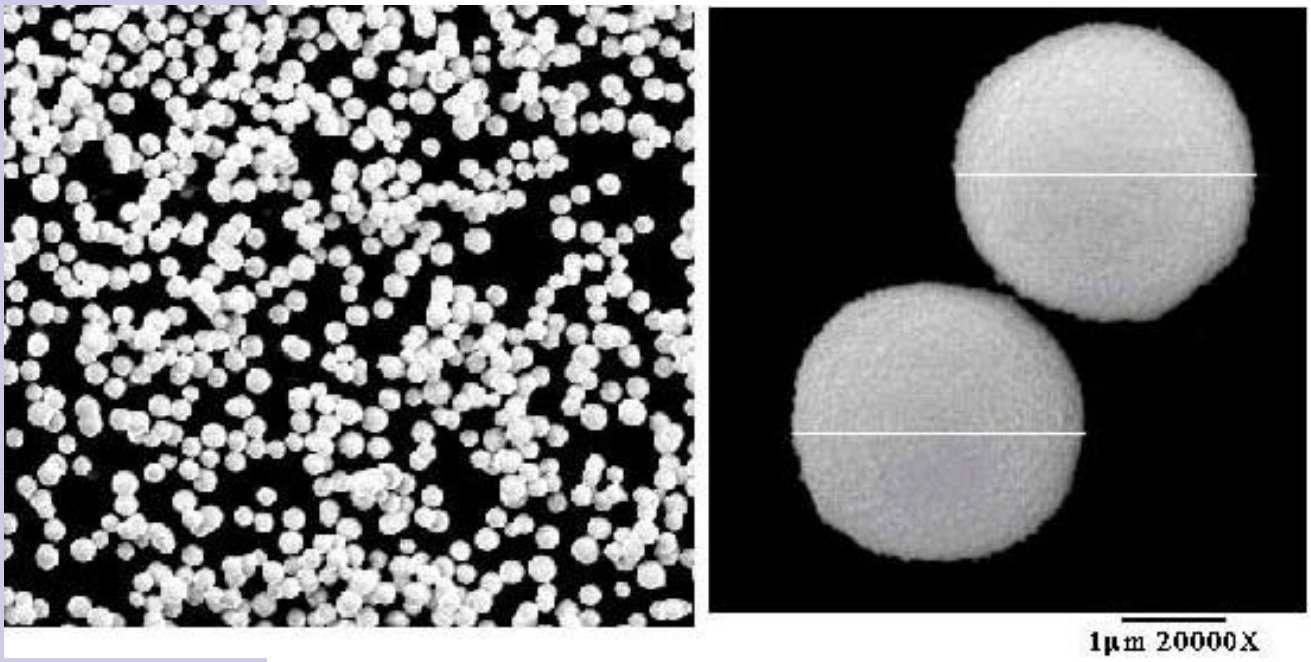
Title: Thermospray Mass Spectrometry Ionization Processes Fundamental Mechanisms for Speciation, Separation and Characterization of Organic Complexants in DOE Wastes

PI: Debra Bostick *Institution:* Oak Ridge National Laboratory

Publication Type: Presentation

Bostick, D. (1999, Aug. 22-26). Separation and speciation of organic complexants in DOE wastes using HPLC on zirconia based stationary phases and thermospray mass spectrometry. Presentation at the National Meeting of the American Chemical Society. New Orleans, LA.

Bostick, D. (1999, Nov. 16). HPLC separation of chelating agents on quaternized polyethyleneimine coated zirconia. Eastern Analytical Symposium, Somerset, NJ.



Electron Micrograph of zirconia particles showing uniform particle size. [see Project #59978]

Bostick, D. (2000, Apr. 24-27). Separation and speciation of organic complexants in DOE wastes using HPLC on zirconia-based stationary phases and thermospray mass spectrometry. 2nd Annual Environmental Management Science Program National Workshop, Atlanta, GA.

Caton, J. E. (1998, Jul. 27-30). Thermospray mass spectrometry ionization processes: Fundamental mechanisms for speciation and characterization of organic complexants in DOE wastes. EMSP Workshop. Chicago, IL.

Project: 60075

Title: Particle Generation by Laser Ablation in Support of Chemical Analysis of High Level Mixed Waste from Plutonium Production Operations

PI: Dr. J. Thomas Dickinson *Institution:* Washington State University

Publication Type: Paper

Dickinson, J. T. (1998, Aug.). Mechanisms for and characterization of particulate generation by laser irradiation of inorganic crystalline materials. DOE-EMSP Workshop on Waste Characterization. Chicago, IL.

Dickinson, J. T. (1998, Jun.). Ejection of droplets and fracture particles from single crystal NaNO 3 during pulsed laser irradiation. Gordon Research Conference on Laser Interaction with Materials.

Dickinson, J. T. (1999, Jun.). UV laser interactions with inorganic single crystals with molecular anions. American Chemical Society. Portland, OR.

Dickinson, J. T. (1999, Mar.). High energy ions from UV laser irradiation of cleaved ionic crystals. American Physical Society March Meeting. Atlanta, GA.

Dickinson, J. T. (1999, Mar.). Laser desorption of energetic ions from single crystal NaNO 3 at 1064 nm. American Physical Society March Meeting. Atlanta, GA.

Dickinson, J. T. (1999, Mar.). The effect of surface treatment on excimer laser induced positive ion desorption in brushite. American Physical Society March Meeting. Atlanta, GA.

Dickinson, J. T. (1999, Mar.). Ultrafast and nanosecond laser induced desorption from ionic solids. American Physical Society March Meeting. Atlanta, GA.

Dickinson, J. T. (1999, May). Laser-induced positive ion and neutral atom/ molecule emission from single crystal CaHPO 4 2H 2 O: The role of radiation induced defects. Materials Research Society. San Francisco, CA.

Dickinson, J. T. (1999, May). Studies of particulate formation by laser ablation in support of chemical analysis of high level mixed waste. American Ceramics Society. Indianapolis, IN.

Hedges, A. L., Mendoza, A., Alexander, M. L., Langford, S.C., & Dickinson, J. T. (1999, Mar.) Investigations of particle formation by laser ablation for elemental analysis. 217th ACS meeting. Anaheim, CA.

Publication Type: Presentation

Alexander, M. L., Langford, S. C., & Dickinson, J. T. (1998, Oct.). Fundamental mechanisms of particulate formation by laser ablation for inductively coupled plasma mass spectrometry (LA/ICP-MS). Presentation at the SPIE East conference. Boston, MA.

Alexander, M. L., Langford, S.C., & Dickinson, J. T. (1999, Mar.). Particle generation by laser ablation in support of chemical analysis of high level mixed waste from plutonium production operations. Invited presentation at the DOE Characterization and Monitoring Sensor Technology (CMST) meeting. Gaithersburg, MD.

Dickinson, J, T. (1999, Jan.). The desorption of energetic ions from ionic crystals. Dept. of Physics, Washington State University. Pullman, WA.

Dickinson, J. T. (1998, Jun.). The laser desorption of ions from ionic crystals. Gordon Conference on Laser Materials Interactions.

Dickinson, J. T. (1998, Nov.). New models of laser desorption and particle formation. Physics Dept. Colloquium. University of Linz, Austria.

Dickinson, J. T. (1998, Oct. - Nov.). Topics in surface dynamics. Guest Lecturer, Institute of Applied Physics. University of Linz, Austria.

Dickinson, J. T. (1998, Oct.). Mechanisms for and characterization of particulate generation by laser irradiation of inorganic crystalline materials. FACS National Meeting. Austin TX.

Dickinson, J. T. (1999, Jan.). The use of lasers in chemical analysis. University of Minho. Braga, Portugal.

Dickinson, J. T. (1999, Jun.). Laser desorption and chemical analysis. Departments of Physics and Chemistry. U. of Heidelberg, Germany.

Dickinson, J. T. (1999, Jun.). The laser desorption of ions from ionic crystals. E-MRS Symposium on Laser Materials Interactions. Strasbourg, France.

Dickinson, J. T. (1999, Jun.). The use of lasers in chemical analysis of toxic materials. Paul Scherrer Institute. Villigen PSI, Switzerland.

Project: 60219

Title: Development of Advanced Electrochemical Emission Spectroscopy for Monitoring Corrosion in Simulated DOE Liquid Waste

PI: Dr. Digby D. MacDonald *Institution:* Pennsylvania State University

Publication Type: Journal

Al-Rifaie, M. & Macdonald, D. D. (2000, in press). On the transients in the thickness of anodic passive films on metals. J. Electrochem. Soc.

Engelhardt, G. R. & Macdonald, D. D. (2000, Mar.). Modeling of corrosion fatigue chemistry in sensitized stainless steel in boiling water reactor environments. CORROSION/2000, Paper No. 00227 (NACE International, Houston, TX.) Orlando, FL.

Macdonald, D. D. & Heaney, D. F. (1999, May). On the photoinhibition of passivity breakdown on iron in chloride-containing solutions. J. Electrochem. Soc. 146(5), 1773-1776.

Macdonald, D. D. (1999). Passivity-the key to our metals-based civilization. Pure Appl. Chem. 71(6), 951-978.

Sikora, E. & Macdonald, D. D. (1999, in press). Electrochemical and photoelectrochemical study of passive films on iron formed in the presence of EDTA. Proc. Int. Symp. Hon. Prof. Norio Sato: Passivity and Localized Corrosion, Electrochemical Society. Princeton, NJ.

Sikora, J., Sikora, E., & Macdonald, D. D. (2000). The electronic structure of the passive film on tungsten. Electrochim. Acta. 45(12), 1875-1883.

Publication Type: Presentation

Liu, J. & Macdonald, D. D. (2000, May 14-19). The passivity of iron in EDTA-containing solutions. Proc. Electrochem. Soc. 198th Meeting. Toronto, Canada.

Macdonald, D. D. & Al-Rifaie, M. (2000, May 14-19). New rate law for the anodic growth of passive films. Proc. Electrochem. Soc. 198th Meeting. Toronto, Canada.

Macdonald, D. D. & Engelhardt, G. R. (2000, Nov. 19-21). The deterministic prediction of localized corrosion damage. Corrosion & Prevention 2000. Auckland, New Zealand.

Macdonald, D. D. (2000, May 14-19). Mechanic analysis by electrochemical impedance spectroscopy. Proc. Electrochem. Soc. 198th Meeting. Toronto, Canada.

Macdonald, D. D. (2000, Nov. 19-21). Fundamental aspects of passivity breakdown. Corrosion & Prevention 2000. Auckland, New Zealand.

Macdonald, D. D. (2000, Nov. 19-21). Mechanistic analysis by electrochemical impedance spectroscopy. Corrosion & Prevention 2000. Auckland, New Zealand.

Macdonald, D. D., Al-Rifaie, M., & Engelhardt, G. R. (2000, Nov. 19-21). Transient growth and reduction of anodic oxide films on metal surfaces. Corrosion & Prevention 2000. Auckland, New Zealand.

Sikora, E. & Macdonald, D. D. (1999). Electrochemical and photoelectrochemical study of passive films on iron formed in the presence of EDTA. 197th Proc. Electrochem. Soc. Meeting. 99-2(484).

Sikora, J., Sikora, E., & MacDonald, D. D. (1999). Nature of the passive film on tungsten. 197th Proc. Electrochem. Soc. Meeting. 99-2(490).

Project: 65421

Title: Correlation of Chemisorption and Electronic Effects for Metal/Oxide Interfaces: Transducing Principles for Temperature-Programmed Gas Microsensors

PI: Dr. Stephen Semancik *Institution:* National Institute of Standards & Technology - Maryland

Publication Type: Patent

Kunt, R. Cavicchi, S. Semancik and T. McAvoy (2001, Aug. 1). Method for Operating a Sensor to Differentiate Between Analytes in a Sample. US #6,095,681

Publication Type: Presentation

Cavicchi, R. E. (1998, Nov. 17). Correlation of chemisorption and electronic effects for metal/oxide interfaces: Transducing principles for temperature programmed gas microsensors. Environmental Management Science Program - Tank Focus Area Workshop. Richland, WA.

Cavicchi, R. E. (1999, Sept. 17-22). Microhotplate gas sensor arrays. Presentation at the SPIE International Symposium on Environmental and Industrial Sensing. Boston, MA.

Ding, J. (1999, Sept. 17-22). Quantification of a single component gas in air with a microhotplate gas sensor using partial least squares techniques. Presentation at the SPIE International Symposium on Industrial and Environmental Sensing. Boston, MA.

McAvoy, T. J. (1999, Aug. 24). Modeling microhotplate gas sensors. Presentation at the ACS National Meeting. New Orleans, LA.

Panchapakesan, B. (1999, Apr. 7). Micromachined array studies of tin oxide films: Nucleation, structure and gas sensing characteristics. MRS Spring National Meeting. San Francisco, CA.

Semancik, S. (1999, Aug. 24). Microarrays as platforms for gas microsensor development and efficient materials research. Presentation at the ACS National Meeting. New Orleans, LA.

Semancik, S. (1999, Sept.). Solid state gas microsensors for environmental and industrial monitoring. Presentation at the SPIE International Symposium on Industrial and Environmental Sensing. Boston, MA.

Walton, R. M. (1999, Jun. 7). Processing methods for selected area film deposition and preparation on microsensor platforms using thermal and potential control. 10th International Conference on Solid-State Sensors and Actuators. Sendai, Japan.

Publication Type: Proceeding

Panchapakesan, B., DeVoe, D. L., Cavicchi, R. E., Walton, R. M., & Semancik, S. (1999, in press). Micromachined array studies of tin oxide films: Nucleation, structure and gas sensing characteristics. Proceedings of the MRS, Spring 1999.

Walton, R., et. al. (1999, Jun.). Processing methods for selected area film deposition and preparation on microsensor platforms using thermal and potential control. Digest 10th International Conference on Solid-State Sensors and Actuators. 1, 676-679. Sendai, Japan.

Project: 65425

Title: Mass Spectrometric Fingerprinting of Tank Waste Using Tunable, Ultrafast Infrared Lasers

PI: Dr. Richard F. Haglund, Jr. *Institution:* Vanderbilt University

Publication Type: Presentation

R. F. Haglund, Jr., (1999, Jun.). The future of tunable, ultrafast lasers in materials analysis and processing. Plenary lecture at the American Society for Mass Spectrometry. Dallas, TX.

Project: 81924 (Renewal of Project No. 60217)

Title: Optical and Microcantilever-Based Sensors for Real-Time In Situ Characterization of High-Level Waste

PI: Dr. Gilbert M. Brown *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Ji, H. - F., Dabestani, R., Brown, G. M., & Hettich, R. L. (1999, Dec.). Optical sensing of cesium using 1,3-alternate calix[4]-mono- and di(anthrylmethyl)aza-crown-6. Photochem. Photobiol. 70(6), 882-886.

Ji, H. -F., Brown, G. M., & Dabestani, R. (1999). Calix[4]arene-based Cs+ selective optical sensor. Chem. Comm. 609.

Ji, H. -F., Dabestani, R., Brown, G. M., & Hettich, R. L. (1999). Spacer length effect on the photoinduced electron transfer fluorescent probe for alkali metal ions. Photochem. Photobiol. 69, 513.

Ji, H.- F., Dabestani, R., & Brown, G. M. (2000, in press). A supramolecular fluorescent probe activated by protons to detect cesium and potassium ions: An integrated logic gate based on photoinduced electron transfer (PET). J. Am. Chem. Soc.

Ji, H.- F., Dabestani, R., Brown, G. M., & Sachleben, R. A. (2000). A new highly selective calix[4]crown-6 fluorescent cesium probe. J. Chem. Soc. Chem. Comm. 833.

Publication Type: Presentation

Ji, H. -F., Dabestani, R., & Brown, G. M. (1998, Aug.). Fluorescence probes for the detection of potassium ions. Presentation at the American Chemical Society National Meeting. Boston, MA.

Project: 81939

Title: Hybrid Micro-Electro-Mechanical Systems (MEMS) for Highly Reliable and Selective Characterization of Tank Waste

PI: Dr. Panos G. Datskos *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Betts, T., Tipple, C., Sepaniak, M., & Datskos, P. G. (2000). Selectivity of chemical sensors based on micro-cantilevers coated with polymeric films. Anal. Chim. Acta. 422, 89.

Datskos, P. G. & Sauers, I. (2000). Detection of 2-mercaptoethanol using microcantilevers. Sensors and Actuators B. 61, 75.

Datskos, P. G. (1999). Chemical detection based on adsorption-induced and photo-induced stresses in MEMS devices. Detection and Remediation Technologies for Mines and Minelike Targets IV, SPIE, 3710, 344.

Fagan, B., Xue, B., Datskos, P. G., & Sepaniak, M. (2000, in press). Modification of micro-cantilever sensors with sol-gels to enhance performance and immobilize chemically selective phases. Talanta.

Headrick, J., Sepaniak, M., Alexandratos, S., & Datskos, P. G. (2000). Chelating scintillation fibers for measurements of 137Cs. Anal. Chem. 72, 1994.

Engineering Science

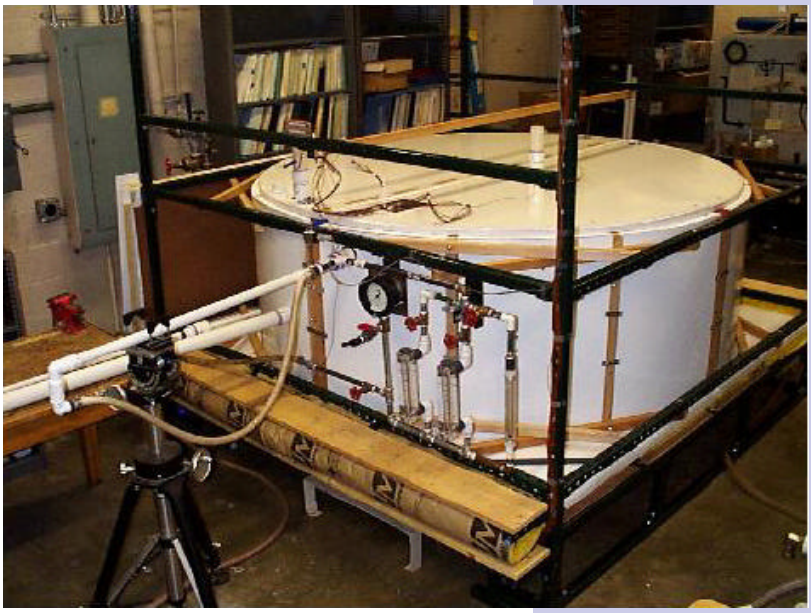
Project: 54656

Title: Mixing Processes in High-Level Waste Tanks
PI: Dr. Per F. Peterson *Institution:* University of California at Berkeley

Publication Type: Presentation

Christensen, J. & Peterson, P. F. (1999, Oct. 3-8). A one-dimensional lagrangian model for large-volume mixing. Accepted for the Ninth International Topical Meeting on Nuclear Reactor Thermal Hydraulics. San Francisco, CA.

Kuhn, S. Z., Lee, C., & Peterson, P. F. (1999, Oct. 3-8). Stratification from buoyancy-driven exchange flow through horizontal partitions in a liquid tank. Accepted for the Ninth International Topical Meeting on Nuclear Reactor Thermal Hydraulics. San Francisco, CA.



Study of Mixing and heat-transfer augmentation by injected jets in a large enclosure. [see Project #54656]

Publication Type: Proceeding

Peterson, P. F. & Gamble, R. E. (1998). Scaling for forced-convection augmentation of heat and mass transfer in large enclosures by injected jets. Transactions of American Nuclear Society. 78, 265-266.

Project: 55294

Title: Superconducting Open-Gradient Magnetic Separation for the Pretreatment of Radioactive or Mixed Waste Vitrification Feeds
PI: Richard D. Doctor *Institution:* Argonne National Laboratory

Publication Type: Paper

Doctor, R. D. (1997, Oct. 24). Superconducting open-gradient magnetic separation for the pre-treatment of radioactive or mixed-waste vitrification feeds. Tenth Symposium on Separation Science and Technology for Energy Applications.

Project: 60451

Title: Mechanics of Bubbles in Sludges and Slurries

PI: Dr. Phillip A. Gauglitz *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Denn, M. M. & Marrucci, G. (1999, Nov. 15). Squeeze flow between finite plates. J. Non-Newtonian Fluid. 87(2-3), 175-178.

Kam, S. I. & Rossen, W. R. (1999, May 15). Anomalous capillary pressure, stress and stability of solids-coated bubbles. J. Colloid Interf. Sci. 213(2), 329-339.

Publication Type: Presentation

Gauglitz, P. A., et. al. (1998, Jun.). Mechanics of bubbles in sludges and slurries: Initial progress. Hanford Technical Exchange. Richland, WA.

Gauglitz, P. A., et. al. (1999, Jan.). Mechanics of bubbles in sludges and slurries. Presented at the Hanford Site Technology Coordinating Group - Tank Subgroup. Richland, WA.

Gauglitz, P. A., Terrones, G., Aardahl, C. L., Mendoza, D. P., & Mahoney, L. A. (1999, Mar. 14-19). Mechanics of bubbles in sludges and slurries: Experi-mental studies and solid mechanics modeling results. Engineering Founda-tion Conference on Rheology in the Minerals Industry II. Oahu, HI.

Publication Type: Report

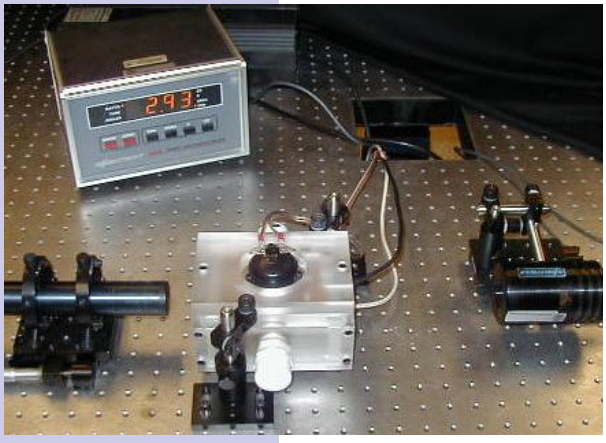
Kam, S. I. (1998). Interactions between bubbles and solids: Three applications. Department of Petroleum and Geosystems Engineering. The University of Texas. Austin, TX.

Project: 65328

Title: Electrically Driven Technologies for Radioactive Aerosol Abatement

PI: Dr. David W. DePaoli

Institution: Oak Ridge National Laboratory



Particle interactions in electric and acoustic fields are studied in a unit reactor. [see Project #65328]

Publication Type: Journal

Carter, J. & Ezekoye, O. A. (2000, in press). Design of an oscillating flow apparatus for the study of low-Reynolds-number particle dynamics. Experiments in Fluids.

Publication Type: Presentation

Ezekoye, O. A. (1998, Nov. 17-18). Electrically driven technologies for radioactive aerosol abate-ment. EMSP/TFA Workshop, Richland, WA.

Schmidt, J. J., et. al. (2000, Apr. 24-27). Electrically driven technologies for radioactive aerosol abatement. Presentation at the 2nd Annual Environmental Management Science Program National Workshop, Atlanta, GA.

Wibowo, Y. W. & Ezekoye, O. A. (1999, Sep.). Computations of sedimentation rates for acoustically enhanced agglomeration. AIChE CCPS Annual International Conference and Workshop on Modeling Consequences of Accidental Releases of Hazardous Materials, San Francisco, CA.

Publication Type: Theses/Dissertations

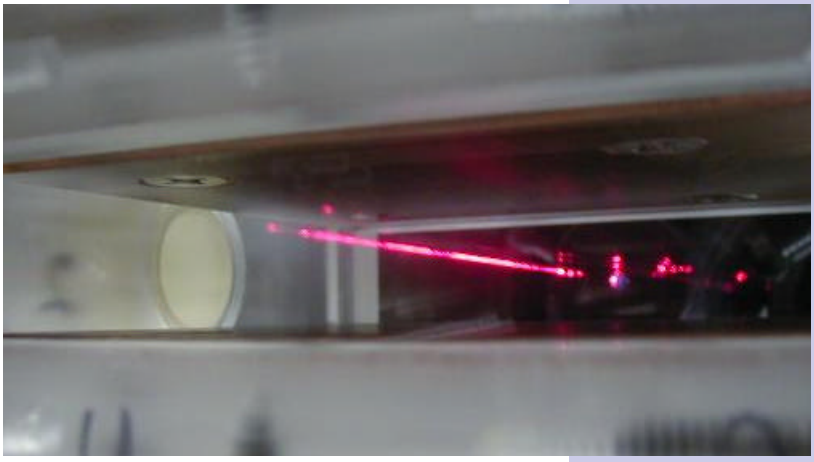
Carter, J. (2000). Study of fluid oscillation and its effect on low Reynolds number particle sedimentation. M. S. Thesis, University of Texas at Austin, TX.

Lakshminarasimhan, K. (in progress). Electrically driven technologies for radioactive aerosol abatement. M. S. Thesis, University of Texas at Austin, TX.

Riahi-Nezhad, C. (projected 2001). Electrically driven technologies for radioactive aerosol abatement. M. S. Thesis, University of Tennessee, Knoxville, TN.

Schmidt, J. J. (2000). Experimental study of electrocoalescence in a unit reactor. M. S. Thesis, University of Texas at Austin, TX.

Experimental apparatus allows testing of the effect of electric and acoustic fields on flowing aerosols in 10-cm (4-inch) square duct. Size distribution and concentration of aerosol are measured to determine effectiveness of agglomeration. [see Project #65328]



Particle size distribution and concentration are measured by light scattering. [see Project #65328]

Project: 65371

Title: Numerical Modeling of Mixing of Chemically Reacting, Non-Newtonian Slurry for Tank Waste Retrieval

PI: Dr. David A. Yuen

Institution: University of Minnesota

Publication Type: Journal

Ten, A. A., Podladchikov, Y. Y., Yuen, D. A., Larsen, T. B., & Malevsky, A. V. (1998). Comparison of mixing properties in convection with the particle-line method. Geophys. Res. Lett. 25(16), 3205-3208.

Ten, A. A., Yuen, D. A. & Podladchikov, Y. Y. (1999, in press). Numerical modeling of mixing of chemically reacting, non-Newtonian slurry for tank waste retrieval. Electronic Geosciences.

Publication Type: Proceeding

Onishi, Y. & Trent, D. S. (1999, Mar. 14-19). Mobilization modeling of erosion-resisting radioactive tank waste. Proceedings of Rheology in the Mineral Industry II, Kahuku, Oahu, HI. Organized by United Engineering Foundation. New York, NY. 45-56.

Onishi, Y., Trent, D. S., Michener, T. E., Van Beek, J. E., & Rieck, C. A. (1999, Jul. 18-23). Simulation of radioactive tank waste mixing with chemical reactions. FEDSM99-7786: Proceedings of 3rd ASME/JSME Joint Fluids Engineering Conference. San Francisco, CA.

Project: 73896 (Renewal of Project No. 55179)

Title: Acoustic Monitor for Liquid-Solid Slurries Measurements at Low Weight Fractions

PI: Dr. Lawrence L. Tavlarides *Institution:* Syracuse University

Publication Type: Journal

Spelt, P. D. M., Norato, M. A., Sangani, A. S., & Tavlarides, L. L. (1999, May). Determination of particle size distributions from acoustic wave propagation measurements. Phys. Fluids. 11(5), 1065-1080.

Geochemistry

Project: 73859 (Renewal of Project No. 55042)

Title: Quantify Silica Reactivity in Subsurface Environments: An Integrated Experimental Study of Quartz and Amorphous Silica to Establish a Baseline for Glass Durability

PI: Dr. Patricia M. Dove *Institution:* Virginia Polytechnic Institute & State Univ.

Publication Type: Other

Dove, P. M. & Icenhower, J. (1997). Kinetic and thermodynamic controls on silica reactivity: An analog for waste disposal media. Commissariat a L' Energie Atomique - Valhro, Ecole D'ete. Invited chapter in Gin, S. (Ed.). Glass: Scientific Research for High Performance Containment.

Publication Type: Presentation

Dove, P. M. (1997, Aug.). Quantifying silica reactivity in subsurface environments: Controls of Reaction Affinity and Solute Matrix on quartz and SIO2 glass. International Nuclear Waste Disposal Conference, CEO-Valhro, France.

Publication Type: Proceeding

Icenhower, J. & Dove, P. M. (1998). The dissolution kinetics of amorphous silica: Structural controls on reactivity (Abstract). International Mineralogical Association Conference. Toronto, Ontario, Canada.

Hydrogeology

Project: 65410

Title: Rapid Migration of Radionuclides Leaked from High-Level Waste Tanks: A Study of Salinity Gradients, Wetted Path Geometry and Water Vapor Transport

PI: Dr. Anderson L. Ward *Institution:* Pacific Northwest National Laboratory

Publication Type: Presentation

Selker, J. S. (1998, Dec. 5-10). Fingered flow from high salinity sources. Presented at the AGU Fall Meetings. San Francisco, CA.

Ward, A. L. & Gee, G. W. (1999, Oct. 31 - Nov. 4). A numerical analysis of wetting front instability induced by infiltration of highly saline fluids. Symposium on Preferential Flow, Soil Science Society of America Annual Meeting. Salt Lake City, UT.

Inorganic Chemistry

Project: 54628

Title: Colloidal Agglomerates in Tank Sludge: Impact on Waste Processing

PI: Dr. Joel M. Tingey *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Liu, J., et. al. (1999, Aug. 22). Characterization of colloidal phases in tank wastes. Abstr. Pap. Am. Chem. S. 218, U1077-U1077, Part 1.

Publication Type: Presentation

Tingey, J. M., Bredt, P. R., & Shekarriz, R. (1999, Mar.). Rheology and settling behavior of Hanford tank wastes and the resulting process streams. Rheology in Mineral Industry II. Kahuku, Oahu, HI.

Tingey, J. M., Bunker, B. C., Graff, G. L., Keefer, K. D., Lea, A. S., & Rector, D. R. (1998, Nov.). Colloidal agglomerates in tank sludge and their impact on waste processing. Materials Research Society Fall Meeting. Boston, MA.

Tingey, J. M., Graff, G. L., & Rector, D. R. (1999, Mar.). Effect of colloidal aggregation on sedimentation and rheology in highly basic, high ionic strength salt solutions. Rheology in Mineral Industry II. Kahuku, Oahu, HI.

Project: 54765

Title: Enhanced Sludge Processing of HLW: Hydrothermal Oxidation of Chromium, Technetium, and Complexants by Nitrate

PI: Dr. Stephen J. Buelow *Institution:* Los Alamos National Laboratory

Publication Type: Journal

Goemans, M. G. E., Funk, T. J., Sedillo, M. A., Buelow, S. J., & Anderson, G. K. (1997). Electrical conductances of aqueous solutions of inorganic nitrates ate 25-505_C and 100-490 bar,î. Journal of Supercritical Fluids. 11, 61-72.

Publication Type: Presentation

Buckley, B., et. al. (1998, Mar. 9-12). Dissolution of chromium oxide under hydrothermal conditions. Presentation at the AIChE 1998 Spring Meeting, New Orleans, LA.

Buelow, S. J. (1996, Oct.). Hydrothermal processing of TRU contaminated wastes. Presentation at the Third International Conference on Oxidation Technologies, Cincinnati, OH.

Buelow, S. J. (1998, Feb. 26-27). Hydrothermal processing of high risk wastes. Presentation at the SCWO Short Course, Supercritical Water Oxidation—Engineering Solutions—Effective Wastewater Treatment and Sludge Management, University of Texas, Austin, TX.

Buelow, S. J., et. al. (1999, Aug. 22-26). Oxidative dissolution of chromium hydroxide by oxygen under hydrothermal conditions. Presentation at the ACS 1999 Fall Meeting, New Orleans, LA.

Ding, Z. Y., et. al. (1998, Jul. 27-30). Enhanced sludge processing of HLW: Hydrothermal Oxidation of Chromium. Presentation at the Environmental Management Science Program Workshop, Rosemont, IL.

Goemans, M. G. E., Butenhoff, T. J., Gloyna, E. F., Anderson, G. K., & Buelow, S. J. (1997, Jun. 22-27). Molecular diffusion of inorganic nitrate species and ketones in subcritcal and supercritical water. Presentation at the Thirteenth Symposium on Thermophysical Properties, Boulder, CO.

Mosher, T., Ding, Z. Y., Buelow, S. J., Foy, B. R., & Robinson, J. M. (1997, Nov. 16-21). Dissolution of chromium oxide in hydrothermal conditions by nitrate. Presentation at the AIChE 1997 Annual Meeting, Los Angeles, CA.

Project: 73778 (Renewal of Project No. 60296)

Title: Research Program to Investigate the Fundamental Chemistry of Technetium

PI: Dr. David K. Shuh *Institution:* Lawrence Berkeley National Laboratory

Publication Type: Presentation

Amonette, A. B., et. al. (1999). The removal of pertechnetate anions from simulated aqueous radioactive tank wastes using supported zero-valent iron. American Chemical Society National Meeting. New Orleans, LA.

Burns, C. J., Fickes, M. G., & Scott, B. L. (1999). Development of synthetic strategies for the preparation of Tc complexes potentially relevant to tank waste and of methodology to immobilize Tc on solid supports. American Chemical Society National Meeting. New Orleans, LA.

Edelstein, N. E. (1998). Aqueous technetium chemistry. U. S. Department of Energy Technetium Workshop. Pacific Northwest National Laboratory. Richland, WA.

Edelstein, N. M. (1999, Sept. 22-25). Technetium chemistry in highly basic solutions. Presentation at the Technetium Chemistry Workshop. Hanford, WA.

Edelstein, N. M., et. al. (1998). Research program to investigate the fundamental chemistry of technetium. Environmental Management Science Program Workshop. Chicago, IL.

Lukens, W. W., Allen, P. G., Bucher, J. J., Edelstein, M. N., & Shuh, D. K. (2000). Radiation chemistry of technetium in highly alkaline solution. Environmental Management Science Program Workshop. Atlanta, GA.

Lukens, W. W., Allen, P. G., Bucher, J. J., Edelstein, M. N., & Shuh, D. K. (2000). Radiation chemistry of technetium in highly alkaline solution. American Chemical Society Meeting. San Francisco, CA.

Lukens, W. W., Bucher, J. J., Edelstein, M. N., & Shuh, D. K. (2000). Radiation chemistry of technetium in highly alkaline solution. American Chemical Society Western Regional Meeting. San Francisco, CA.

Lukens, W. W., et. al. (1999). The chemistry of reduced technetium in base. American Chemical Society National Meeting. New Orleans, LA.

Mallouk, T. E., et. al. (2000). Some chemical solutions to the remediation of aqueous wastes containing cesium, technetium, and other toxic metal ions. Environmental Management Science Program Workshop. Atlanta, GA.

Shuh, D. K. (1998). Radionuclide environmental chemistry. Department of Chemistry. Foothill College. Los Altos, CA.

Shuh, D. K. (1998). Synchrotron radiation techniques for the investigation of environmental materials science. MRS Spring Meeting. San Francisco, CA.

Shuh, D. K. (1998). Technetium chemistry in cement waste forms. U. S. Department of Energy Technetium Workshop. Pacific Northwest National Laboratory. Richland, WA.

Project: 73832 (Renewal of Project No. 55229)

Title: The NOx System in Homogeneous and Heterogeneous Nuclear Waste

PI: Dr. Dan Meisel *Institution:* University of Notre Dame

Publication Type: Journal

Cook, A. R., et. al. (2001, Mar. 16). Reducing radicals in nitrate solutions: The NO3 2- system revisited. J. Phys. Chem. B, 105. Web Edition.

Dimitrijevic, N. M., Henglein, A., & Meisel, D. (1999). Charge separation across the silica nanoparticle/ water interface. J. Phys. Chem. B. 103, 7073-7076.

Fessenden, R. W., Meisel, D., & Camaioni, D. M. (2000). Addition of oxide radical ions (O-) to nitrite and oxide ions (O2-) to nitrogen dioxide. J. Am. Chem. Soc. 122, 3773-3774.

Schatz, T., Cook, A., & Meisel, D. (1999). Capture of charge carriers at the silica nanoparticle - water interface. J. Phys. Chem. B, 103. 10209-10213.

Publication Type: Presentation

Schatz, T., Cook, A. R., & Meisel, D. (1998). Charge carrier transfer across the silica nanoparticle / water interface. J. Phys. Chem. B. 102, 7225-7230.

Publication Type: Proceeding

Babad, H. & Camaioni, D. M. (2000, Feb. 27-Mar. 2). The aging of organic chemicals in Hanford high-level wastes. Tucson, AZ.

Meisel, D. (1997). Semiconductor nanoclusters, physical, chemical, and catalytic aspects. In Kamat, P. V. & Meisel, D. (Eds.), Studies in Surface Science and Catalysis. 103, 79-97.

Meisel, D. (2000). Radiation induced charge carriers in aqueous suspensions of nanoparticles. Proceedings of the Trombay Symposium on Radiation and Photochemistry. II, 271-279.

Meisel, D., Camaioni, D., & Orlando, T. (2001). Radiation and chemistry in nuclear waste: The nox sytem and organic aging. In Eller, G. & Heineman, W. R. (Eds.), ACS Symposium Series 778. 342-361.

Meisel, D., Cook, A., Camaioni, D., & Orlando, T. (1997). Photoelectrochemistry. In Rajeshwar, K., Peter, L. M., Fujishima, A., Meissner, D., & Tomkiewicz, M. (Eds.), The Electrochemical Society Pub. 97-20, 350-357.

Orlando, T. & Meisel, D. (2001). Radiation-induced processes in aqueous suspensions of nanoparticles and nanoscale water films. In Eller, G. & Heineman, W. R. (Eds.), ACS Symposium Series 778. 284-296.

Materials Science

Project: 54773

Title: Microstructural Properties of High-Level Waste Concentrates and Gels with Raman and Infrared Spectroscopies

PI: Dr. Stephen F. Agnew *Institution:* Los Alamos National Laboratory

Publication Type: Presentation

Agnew, S. (1997, Jun. 18-21). IR and raman studies of high level waste concentrates. Presentation at the 52nd Northwest Regional ACS Meeting, Moscow, ID.

Johnston, C. (1999, Mar. 11). Microstructural properties of high level waste concentrates and gels with raman and infrared spectroscopies. Presentation at the CMST-CP annual review conference, Gaithersburg, MD.

Project: 55188

Title: Chemical Decomposition of High-Level Nuclear Waste Storage/Disposal Glasses Under Irradiation

PI: Dr. David L. Griscom *Institution:* Naval Research Laboratory

Publication Type: Journal

Griscom, D. L., Beltran-Lopez, V., Merzbacher, C. I., & Bolden, E. (1999, Jul. 10-15). Selected papers from the 18th International Congress on Glass, San Francisco, CA. J. Non-Cryst. Solids, 253, 1-22.

Griscom, D. L., et. al. (1998). On the structure and radiation chemistry of iron phosphate glasses: New insights from electron spin resonance, Mossbauer, and evolved-gas mass spectroscopy. Nucl. Inst. & Methods B, 141, 600-615.

Griscom, D. L., Merzbacher, C. I., Weeks, R. A., & Zuhr, R. A. (1999). Electron spin resonance studies of defect centers induced in a high-level nuclear waste glass simulant by gamma-irradiation and ion-implantion. J. Non-Cryst. Solids. 258, 34-47.

Project: 55367

Title: Investigation of Microscopic Radiation Damage in Waste Forms Using ODNMR and AEM Techniques

PI: Dr. Guokui Liu *Institution:* Argonne National Laboratory

Publication Type: Journal

Liu, G. K., et. al. (1998). Crystal-field splitting, magnetic interaction, and vibronic excitations of 244Cm in YP04 and LuP04. J. Phys. Chem. 109, 6800-6808.

Liu, G. K., et. al. (2000). Studies of local structure of Cm3+ in borosilicate glass using laser and x-ray spectroscopic methods and computational modeling. J. Chem. Phys. 112, 1489-1496.

Liu, G. K., Li, S. T., Beitz, J. V., & Abraham, M. M. (1998). Effects of self-radiation damage on electronic properties of 244CM3+ in an orthophosphate crystal of YP04. J. Alloys & Compounds. 271/273, 872-875.

Liu, G. K., Zhorin, V. V., Li, S. T., & Beitz, J. V. (2000). Crystal field analysis and Monte Carlo simulation of lattice disordering for Cm3+ in YP04 and LuP04. J. Chem. Phys. 112, 373-382.

Zhorin, V. V. & Liu, G. K. (1998). Modeling crystal-field interaction for f-elements in LaC13. J. Alloys and Compounds 275/277, 137-141.

Publication Type: Proceeding

G. K. Liu, et. al. (1998). Scientific basis for nuclear waste management XXI. MRS Sym. Pro. V506, 921.

Liu, G. K., et. al. (1998). Self-radiation induced anisotropic structure damage in 244Cm-doped orthophosphate LuP04. Scientific Basis for Nuclear Waste Management XXI, Mat. Res. Soc. Symp. Proc. 506, 921-922.

Project: 59827

Title: The Influence of Radiation and Multivalent Cation Additions on Phase Separation and Crystallization of Glass

PI: Dr. Michael C. Weinberg *Institution:* University of Arizona

Publication Type: Journal

Burgner, L. L. & Weinberg, M. C. (2000, Jan.). Crystal nucleation rates in a Na 2 O-SiO 2 glass. J. Non-Cryst. Solids. 261(1-3), 163-168.

Publication Type: Paper

Jeoung, J. S., Poisl, W. H., Weinberg, M. C., Smith, G. L., & Li, H. (1999). Effect of iron oxidation state on immiscibility temperature in sodium silicate glass. Amer. Ceram. Soc. Bull. 78(4), 205.

Project: 65422

Title: Modeling of Spinel Settling in Waste Glass Melter

PI: Dr. Pavel Hrma *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Casler, D. G. & Hrma, P. (1999). Nonisothermal kinetics of spinel crystallization in a HLW glass. Mat. Res. Soc. Proc. 556, 255-262.

Hrma, P., Vienna, J. D., Crum, J. V., Piepel, G. F., & Mika, M. (2000). Liquidus temperature of high-level waste borosilicate glasses with spinel primary phase. Mat. Res. Soc. Proc. 608, 671-676.

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Publication Type: Paper

Mika, M., Crum, J. V., & Hrma, P. (1999). Spinel precipitation in high-level waste glass. Proceedings of the 5th ESG Conference. Prague, Czech Republic.

Publication Type: Presentation

Hrma, P. & Alton, J. (2001). Dissolution and growth of spinel crystals in high-level waste glass: Diffusion coefficient and boundary layer thickness. ICEM ’01. The 8th International Conference on Radioactive Waste Management and Environmental Remediation. Bruges, Belgium.

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Publication Type: Proceeding

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Publication Type: Report

Hrma, P. (1999). Modeling of spinel settling in waste glass melter. In Science to Support DOE Site Cleanup. Pacific Northwest National Laboratory. PNNL-12208 UC-2000.

Publication Type: Theses/Dissertations

Matyas, J. (2001). Description of the behavior of multitude particles in non-isothermal convective melting space. PhD. Dissertation. Laboratory of Inorganic Materials. Prague, Czech Republic.

Project: 73748 (Renewal of Project No. 60345)

Title: New Metal Niobate and Silicotitanate Ion Exchangers: Development and Characterization

PI: Yali Su *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Nyman M., et. al. (1999, in press). Synthesis and characterization of a new microporous Cs-Ti-Si-O-H2O ion exchanger. Chemistry of Materials.

Nyman, M., et. al. (1999, Mar. 21). Synthesis, characterization, ion exchange, and ion selectivity of novel microporous Cs-Na-Si-Ti-X-O-H2O (X=transition metal) materials. Abstr. Pap. Am. Chem. S. 217, U924-U924, Part 1.

Xu, H. W., Navrotsky, A., Nyman, M. D., & Nenoff, T. M. (2000, Mar.). Thermochemistry of microporous silicotitanate phases in the Na2O-Cs2O-SiO2-TiO2-H2O system. J. Mater. Res. 15(3), 815-823.

Publication Type: Patent

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Publication Type: Presentation

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Balmer, M. L., et. al. (1999, Apr. 25-28). Ceramic wasteforms from Cs-loaded crystalline silicotitanates. 101th Annual Meeting of the American Ceramic Society. Indianapolis, IN.

Nyman, M. D. & Nenoff, T. M. (1999, Jun.). Selective inorganic crystalline ion exchange materials for cesium and strontium. United Engineering Foundation and AIChE.

Nyman, M. D., et. al. (1998). CSTs: Stability and use as alternative waste forms. Mat. Res. Soc. Fall Meeting.

Nyman, M. D., et. al. (1999). Hydrothermal synthesis of Cs-Ti-Si-O phases as alternative waste forms for Cs-loaded CST ion exchangers. 1999 Spring American Chemical Society Meeting. Anaheim, CA.

Su, Y., et. al. (1998). Evaluation of thermally converted silicotitanate waste forms II. Mat. Res. Soc. Fall Meeting.

Xu, H., et. al. (1999, Apr. 25-28). Thermo-chemistry of crystalline silicotitanate phases in the Cs2O-Na2O-SiO2-TiO2-H2O system. 101st Annual Meeting of the American Ceramic Society. Indianapolis, IN.

Publication Type: Proceeding

Nyman, M. D., et. al. (1998). CSTs: Stability and use as alternative waste forms. Proc. Mat. Res. Soc. Fall Meeting.

Project: 73750 (Renewal of Project No. 54672)

Title: Radiation Effects in Nuclear Waste Materials

PI: Dr. William J. Weber *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Begg, B. D., Hess, N. J., & Weber, W. J. (2000, Apr.). XAS and XRD study of annealed Pu-238- and Pu-239-substituted zircons (Zr0.92Pu0.08SiO4). J. Nucl. Mater. 278(2-3), 212-224.

Corrales, L. R. (1999, Jun. 21). The formation and migration energetics of radical defects in silica polymorphs. Abstr. Pap. Am. Chem. S. 217, U293-U293, Part 2.

Gorretta, K. C., et. al. (1999). Solid-particle erosion of Portland cement and concrete. Wear 224, 106-112.

Hess, N. J., Weber, W. J., & Conradson, S. D. (1998). U and Pu LIII XAFS of Pu-doped glass and ceramic waste forms. Journal of Alloys and Compounds, 271-273, 240-243.

Hess, N. J., Weber, W. J., & Conradson, S. D. (1998). X-ray absorption fine structure of aged, Pu-doped glass and ceramic waste forms. Journal of Nuclear Materials. 254, 175-184.

Park, B., Weber, W. J., & Corrales, L. R. (2000). Molecular dynamics study of the threshold displacement energy in MgO. Nucl. Instrum. and Methods, B, 166-167, 357-363.

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Thevuthasan, S., Jiang, W., & Young, J. S. (2000, Mar.). Investigation of thermal recovery behavior in hydrogen-implanted SrTiO3 using high energy ion beam techniques. Nucl. Instrum. Meth. B. 161, 544-548.

Weber, W. J., Ewing, R. C., & Meldrum, A. (1997). The kinetics of alpha-decay-induced amorphization in zircon and apatite containing weapons-grade plutonium or other actinides. Journal of Nuclear Materials. 250, 147-155.

Williford, R. E., Begg, B. D., Weber, W. J., & Hess, N. J. (2000, Apr.). Computer simulation of Pu 3+ and Pu 4+ substitutions in zircon. J. Nucl Mater. 278(2-3), 207-211.

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Publication Type: Other

Begg, B. D., et. al. (1999, in press). Heavy-ion irradiation effects in pyrochlores. Smith, G. L., Chandler, G. T., & Mobasher, B. (Eds.), Waste Management Science and Technology in the Ceramic and Nuclear Industries. The American Ceramic Society. Westerville, OH.

Chen, X., Birtcher, R. C., & Donnelly, S. E. (1999). Bubble formation and growth in glasses. Zinkle, S. J., Ewing, R. C., Lucas, G. E., & Williams, J. S. (Eds.). Microstructural Processes in Irradiated Materials. Mater. Res. Soc. Symp. Proc. 540. Warrendale, PA. 331-336.

Corrales, L. R., Song, J., VanGinhoven, R. M., & Jonsson, H. (2000). A comparative study of oxygen vacancy migration pathways in crystalline polymorphs of silica. Chandler, G. T. & Feng, X. (Eds). Environmental Issues and Waste Management Technologies in the Ceramic and Nuclear Industries V, Ceramics Transactions, Westerville, OH. 107, 139-150.

Corrales, L. R., Song, J., VanGinhoven, R. M., & Jónsson, H. (1999, in press). Vacancy migration and excitons in silica polymorphs. Smith, G. L., Chandler, G. T., & Mobasher, B. (Eds.). Mater. Waste Management Science and Technology in the Ceramic and Nuclear Industries. The American Ceramic Society. Westerville, OH.

Publication Type: Paper

Williford, R. E. & Weber, W. J. (1999, Apr. 25-28). Defect formation and migration energetics in disordered Gd2Ti2O7. The 101st Meeting of The American Ceramic Society. Indianapolis, IN.

Publication Type: Presentation

Begg, B. D., et. al. (1999, Apr. 25-28). Heavy-ion irradiation effects in pyrochlores. The 101st Meeting of The American Ceramic Society. Indianapolis, IN.

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Chen, X., Birtcher, R. C., & Donnelly, S. E. (1998, Nov. 30 - Dec. 4). Bubble formation and growth in nuclear waste glasses. Materials Research Society Annual Meeting. Boston, MA.

Corrales, L. R. & Song, J. (1997, Sept.). Molecular dynamics simulations of excitons in glasses. CEA/VALHRO Summer School. Mejannes le Clap, France.

Corrales, L. R. (1997, Oct.). Lattice theories and molecular dynamics simulations of glasses. Department of Chemistry, University of Maryland. College Park, MD.

Corrales, L. R. (1997, Oct.). Molecular dynamics simulations of defects and excitons in glasses. American Ceramics Society, Glass and Optical Materials Division Meeting. Williamsburg, VA.

Corrales, L. R., Song, J., VanGinhoven, R. M., & Jónsson, H. (1999, Apr. 25-28). The formation and migration energetics of radical defects in silica polymorphs. Invited presentation at the 101st Meeting of The American Ceramic Society. Indianapolis, IN.

Corrales, L. R., Song, J., VanGinhoven, R. M., & Jónsson, H. (1999, Mar. 21-25). Migration of oxygen vacancy radical defects and self-trapped excitons in silica. Invited presentation at the 217th American Chemical Society Meeting. Anaheim, CA.

Corrales, L. R., VanGinhoven, R. M., Song, J., & Jónsson, H. (1998, Nov. 30 - Dec. 4). Vacancy migration barrier energetics and pathways in silica. Materials Research Society Annual Meeting. Boston, MA.

Devanathan, R., Weber, W. J., & Boatner, L. A. (1997, Dec. 1-5). Response of zircon to electron and Ne + irradiation. Materials Research Society Annual Meeting. Boston, MA.

Devanathan, R., Weber, W. J., & Williford, R. E. (1998, Nov. 30 - Dec. 4). Amorphization of Gd2Ti2O7 by energetic heavy ion irradiation. Materials Research Society Annual Meeting. Boston, MA.

Fortner, J. A., Hanchar, J. M., Badyal, Y., Price, D. L., & Weber, W. J. (1998, Nov. 30 - Dec. 4). Structural analysis of a completely amorphous 238 Pu-doped zircon by neutron diffraction. Materials Research Society Annual Meeting. Boston, MA.

Hess, N. J., Maupin, G. D., & Weber, W. J. (1998, Nov. 30 - Dec. 4). Spectroscopic studies of gamma-irradiated glass waste forms. Materials Research Society Annual Meeting, Boston, MA.

Hess, N. J., Weber, W. J., & Conradson, S. D. (1997, Sept. 21-26). U and Pu LIII XAFS of Pu-doped glass and ceramic waste forms. International Conference on Actinides ‘97. Baden-Baden, Germany.

Song, J. & Corrales L. R. (1998, Mar. 16-20). Simulation of exciton processes in networked materials. March APS National Meeting. Anaheim, CA.

Song, J., Corrales, L. R., & Jónsson, H. (1998, Nov. 30 - Dec. 4). Exploring the excited states of vacancy defects in silica. Materials Research Society Annual Meeting. Boston, MA.

Thevuthasan, S., Jiang, W., McCready, D. E., & Weber, W. J. (1998, Nov. 30 - Dec. 4). Damage accumulation and thermal recovery in SrTiO3 implanted with various ions. Materials Research Society Annual Meeting. Boston, MA.

Weber, W. J. & Corrales, L. R. (1998, July 27-30). Radiation effects in nuclear waste forms. DOE Environmental Management Science Program Scientific Workshop. Rosemont, IL.

Weber, W. J. & Devanathan, R. (1998, May 4-6). Effects of alpha decay on crystalline ceramic waste forms. American Ceramic Society Meeting. Cincinnati, OH.

Weber, W. J. (1988, July 27-30). EMSP projects in materials science. DOE Environmental Management Science Program Scientific Workshop. Rosemont, IL.

Weber, W. J. (1997, Dec. 1). Radiation effects in glass and ceramic waste forms. Invited presentation at the Massachusetts Institute of Technology. Cambridge, MA.

Weber, W. J. (1997, Dec. 11). Radiation effects in glass waste forms. Invited presentation at Argonne National Laboratory. Argonne, IL.

Weber, W. J. (1997, Feb. 20). Radiation effects from the incorporation of plutonium in glasses and ceramics. Invited presentation at Los Alamos National Laboratory. Los Alamos, NM.

Weber, W. J. (1998, Apr. 19-22). Effects of radiation on solid nuclear waste forms. Invited plenary lecture at the DOE Workshop on Research Needs and Opportunities in Radiation Chemistry. Chesterton, IN.

Weber, W. J. (1998, Apr. 3-4). Radiation effects from alpha decay in nuclear waste ceramics. Invited plenary lecture at the American Nuclear Society Northern Student Conference. Ann Arbor, MI.

Weber, W. J. (1998, Jan. 8). Radiation effects in crystalline waste form phases. Invited presentation at the Idaho National Engineering and Environmental Laboratory. Idaho Falls, ID.

Weber, W. J., et. al. (1998, Nov. 30 - Dec. 4). The effect of temperature and recoil spectra on amorphization in zircon. Materials Research Society Annual Meeting. Boston, MA.

Weber, W. J., Ewing, R. C., & Meldrum, A. (1998, Mar. 30 - Apr. 3). Radiation effects in nuclear waste ceramics. American Chemical Society Annual Meeting. Dallas, TX.

Weber, W. J., Hess, N. J., Conradson, S. D., & Vienna, J. D. (1997, Aug. 25-27). Self-radiation effects in glass and ceramic waste forms for the stabilization and disposition of plutonium. Topical Conference on Plutonium Futures - The Science. Santa Fe, NM.

Williford, R. E., Devanathan, R. & Weber, W. J. (1997, Sept. 14-19). Computer simulation of displacement threshold energies for several ceramic materials. 9th International Conference on Radiation Effects in Insulators. Knoxville, TN.

Williford, R. E., Weber, W. J., Devanathan, R., & Gale, J. D. (1998, Nov. 30 - Dec. 4). Oxygen vacancy migration in Gd2(Ti,Zr)2O7 pyrochlores. Materials Research Society Annual Meeting. Boston, MA.

Publication Type: Proceeding

Corrales, L. R. & Song, J. (1998). Semi-empirical methodology to simulate exciton processes in glasses. Proceeds of the CEA/VALRHO Summer School on Glass: Scientific Research for High Performance Containment. CEA/Valrhô, Bagnols-sur-Cèze, France, 218-227.

Corrales, L. R., VanGinhoven, R. M., Song, J., & Jónsson, H. (1999). Vacancy migration barrier energetics and pathways in silica. Bulatov, V. V., Diaz de la Rubia, T., Phillips, R., Kaxiras, E., & Ghoniem, N. (Eds.) Multiscale Modeling of Materials. Mater. Res. Soc. Symp. Proc. 538, Warrendale, PA. 317-321.

Devanathan, R., Weber, W. J., & Boatner, L. A.. (1998). Response of zircon to electron and Ne + irradiation. Ma, E., Bellon, P., Atzmon, M., & Trivedi, R. (Eds.) Phase Transformations and Systems Driven far from Equilibrium. Mater. Res. Soc. Symp. Proc. 481, Warrendale, PA. 419-424.

Fortner, J. A., Hanchar, J. M., Badyal, Y., Price, D. L., & Weber, W. J. (1999, in press). Structural analysis of a completely amorphous 238 Pu-doped zircon by neutron diffraction. Zinkle, S. J., Ewing, R. C., Lucas, G. E., & Williams, J. S. (Eds.). Microstructural Processes in Irradiated Materials. Mater. Res. Soc. Symp. Proc. 540, Warrendale, PA.

Heinisch, H. L., Williford, R. E. & Weber, W. J. (1998, Nov. 30 - Dec. 4). Computer simulations of irradiation-induced defect accumulation and amorphization in zircon. Materials Research Society Annual Meeting. Boston, MA.

Hess, N. J., Weber, W. J., & Conradson, S. D. (1998). X-ray absorption fine structure of aged, Pu-doped glass and ceramic waste forms. McKinley, I. G. & McCombie, C. (Eds.), Scientific Basis for Nuclear Waste Management XXI. Mater. Res. Soc. Symp. Proc. 506, Warrendale, PA. 169-176.

Hess, N. J., Weber, W. J., & Conradson, S. D. (1997, Sept. 28 - Oct. 3). X-ray absorption fine structure of aged, Pu-doped glass and ceramic waste forms. MRS Symposium, Scientific Basis for Nuclear Waste Management XXI. Davos, Switzerland.

Thevuthasan, S., Jiang, W., McCready, D. E., & Weber, W. J. (1999, in press). Damage accumulation and thermal recovery in SrTiO3 implanted with various ions. Zinkle, S. J., Ewing, R. C., Lucas, G. E., & Williams, J. S. (Eds.), Microstructural Processes in Irradiated Materials. Mater. Res. Soc. Symp. Proc. 540, Warrendale, PA.

Weber, W. J., et. al. (1999, in press). The effect of temperature and recoil spectra on amorphization in zircon. Zinkle, S. J., Ewing, R. C., Lucas, G. E., & Williams, J. S. (Eds.), Microstructural Processes in Irradiated Materials. Mater. Res. Soc. Symp. Proc. 540, Warrendale, PA.

Publication Type: Report

Weber, W. J. & Corrales, L. R. (1997). Radiation effects in nuclear waste materials. Science to Support DOE Site Cleanup: The Pacific Northwest National Laboratory Environmental Management Science Program Awards. PNNL-11589, Pacific Northwest National Laboratory. Richland, WA. 43-52.

Weber, W. J. & Corrales, L. R. (1998). Radiation effects in nuclear waste materials. Science to Support DOE Site Cleanup: The Pacific Northwest National Laboratory Environmental Management Science Program Awards (PNNL-11889, Pacific Northwest National Laboratory, Richland, WA.). 1.107-1.126.

Weber, W. J. & Corrales, L. R. (1998). Radiation effects in nuclear waste materials. Science to Support DOE Site Cleanup: The Pacific Northwest National Laboratory Environmental Management Science Program Awards. PNNL-11889, Pacific Northwest National Laboratory. Richland, WA. 1.107-1.126.

Weber, W. J., Corrales, L. R., Birtcher, R. C., & Nastasi, M. (1998). Radiation effects in nuclear waste materials. Environmental Management Science Program Workshop (CONF-980736, U. S. Department of Energy, Office of Science and Technical Information, Oak Ridge, TN.). 115-117.

Weber, W. J., Hess, N. J., Conradson, S. D., & Vienna, J. D. (1997). Self-radiation effects in glass and ceramic waste forms for the stabilization and disposition of plutonium. Plutonium Futures - The Science. LA-13338-C, Los Alamos National Laboratory. Los Alamos, NM. 25-26.

Project: 73762 (Renewal of Project No. 54691)

Title: Radiation Effects on Sorption and Mobilization of Radionuclides During Transport Through the Geosphere

PI: Dr. Lu-Min Wang *Institution:* University of Michigan

Publication Type: Journal

Gu, B. X., et. al. (2000). The effect of H+ irradiation on the Cs ion exchange capacity of zeolite-NaY. J. Materials Chemistry. 10, 2610-2616.

Gu, B. X., Wang, L. M., & Ewing, R. C. (2000, Mar.). The effect of amorphization on the Cs ion exchange and retention capacity of zeolite-NaY. J. Nucl. Mater. 278, 64-72.

Nyman, M., et. al. (2000). Integrated experimental and computational methods for structure determination and characterization of a new, highly stable cesium silicotitanate phase, Cs2TiSi6O15 (SNL-A). Chemistry of Materials. 12, 3449-3458.

Nyman, M., Gu, B. X., Wang, L. M., Ewing, R. C., & Neoff, T. M. (2000). Synthesis and characterization of a new microporous cesium silicotitanate (SNL-B) molecular sieve. Microporous Materials. 40, 115-125.

Wang, L. M. (1998). Application of advanced transmission electron microscopy techniques in the study of radiation effects in insulators. Nuclear Instruments and Methods in Physics Research B. 141, 312-325.

Wang, L. M., Wang, S. X., Gong, W. L., & Ewing, R. C. (1998). Temperature dependence of Kr ion-induced amorphization of mica minerals. Nuclear Instruments and Methods in Physics Research B. 141, 501-508.

Wang, S. X., Wang, L. M., & Ewing, R. C. (2000). Electron and ion irradiation of zeolites. J. Nucl. Mater. 278, 233-241.

Publication Type: Proceeding

Gu, B. X., Wang, L. M., Simpson, P. A., Minc, L. D., & Ewing, R. C. (2000, in press). Radiation and thermal effects in zeolite-NaY. Smith, R. W. & Shoesmith, D. W. (Eds.). Scientific Basis for Nuclear Waste Management XXIII, Material Research Society. Warrendale, PA.

Gu, B. X., Wang, S. X., Wang, L. M., & Ewing, R. C. (1999, Aug. 29 - Sept. 3). Radiation and thermal effects on the structure and ion-exchange/retention capacity of zeolites. Proceedings of the International Conference on the Future Nuclear Systems-Global '99. American Nuclear Society. Jackson Hole, WY.

Wang, L. M. & Ewing, R. C. (1998, Aug. 31 - Sep. 4). Transmission electron microscopy study of radiation effects in materials for nuclear waste disposal. Benavides, H. A. C. & Yacaman, M. J. (Eds.) Electron Microscopy 1998, Proceedings of the 14th International Congress on Electron Microscopy. 2, 825-826. Cancun, Mexico.

Wang, L. M., Wang, X. M., & Ewing, R. C. (1998, May 11-14). Radiation effects in zeolite: Relevance to near-field containment. Proceedings of the 9th Annual International High-Level Radioactive Waste Management Conference, American Nuclear Society. Las Vegas, NV. 772-774.

Wang, S. X., Wang, L. M., & Ewing, R. C. (1999). Electron irradiation of zeolites. Materials Research Society Symposia Proceedings. 540, 361-366.

Project: 73976 (Renewal of Project No. 55110)

Title: Iron Phosphate Glasses: An Alternative for Vitrifying Certain Nuclear Wastes
PI: Dr. Delbert E. Day *Institution:* University of Missouri-Rolla

Publication Type: Journal

Badyal, Y., et. al. (2000). The effects of uranium oxide high-level waste on the structure of iron phosphate glasses. MRS 556, 297.

Booth, C. S., et. al. (1999). Oxygen and phosphorus coordination around iron in iron-phosphate glasses with U02 or Na2 O and crystalline ferric ferrous pyrophosphate. J. Mat. Res. 14, 2628.

Chen, F. & Day, D. E. (1999). Corrosion of selected refractories by iron phosphate melts. Environment Issues and Waste Management Technologies IV: Ceramic Transactions. 93, 213.

Day, D. E. (1997). Structural features of iron-phosphate glasses. J. Non-Cryst. Solids. 222, 144.

Day, D. E. (1997). Structural study of iron phosphate glasses. Phys. Chem. Glasses. 38, 74.

Day, D. E. (1998). Chemically durable iron phophate glass wasteforms. J. Non-Cryst. Solids. 241, 1.

Day, D. E. (1998). On the structure and radiation chemistry of iron phosphate glasses: New insights from electron spin resonance and evolved gas mass spectroscopy. Nucl. Inst. Meth. Phys. Res. B. 141, 600.

Day, D. E. (1998). Redox characteristics and structural properties of iron phosphate glasses: A potential host matrix for vitrifying high level nuclear waste. Ceramic Transactions. 87, 261.

Day, D. E. (1999). Effects of nuclear waste components on redox equilibria, structural features, and crystallization characteristics of iron phosphate glasses. Environment Issues and Waste Management Technologies IV: Ceramic Transactions. 93, 195.

Day, D. E. (1999). Iron redox equilibria and crystallization of iron phosphate glasses. Environment Issues and Waste Management Technologies IV: Ceramic Transactions. 93, 187.

Fang, X., Ray, C. S., Marasinghe, G. K., & Day, D. E. (2000). Properties of mixed Na2 O and K2 O iron phosphate glasses. J. Non-Cryst. Solids 263, 293.

Karabulut, M., et. al. (1999). X-ray photoelectron and mossbauer spectroscopic studies of iron phosphate glasses containing U, Cs, and Bi. J. Non-Cryst. Solids. 249, 106.

Karabulut, M., et. al. (2000). A high-energy x-ray and neutron scattering study of iron-phosphate glasses containing uranium. J. Appl. Phys. 87, 2185.

Marasinghe, G. K., et. al. (2000). Properties and structure of vitrified iron phosphate nuclear wasteforms. J. Non-Cryst. Solids. 263, 146.

Marasinghe, G. K., et. al. (2000). Vitrified iron phosphate nuclear wasteforms containing multiple waste components. Environment Issues and Waste Management Technologies V: Ceramic Transactions. 107, 115.

Mesko, M. G. & Day, D. E. (1999). Immobilization of spent nuclear fuel in iron phosphate glass. J. Nuclear Matls. 273, 27-36.

Mesko, M. G., Day, D. E., & Bunker, B. C. (2000). Immobilization of CsCl and SrF2 in iron phosphate glass. Environment Issues and Waste Management Technologies V: Ceramic Transactions. 107.

Mogus-Milankovic, A., Day, D. E., & Santic, B. (1999). DC conductivity and polarization in iron phosphate glasses. Phys. Chem. Glasses 40 (2),69-74.

Mogus-Milankovic, A., Santic, B., Pivac, B., & Day, D. E. (1999). TSC and DC conductivity for cesium iron phosphate glasses. Phys. Chem. Glasses 40(6), 305-310.

Ray, C. S., Fang, X., Karabulut, M., Marasinghe, G. K., & Day, D. E. (1999). Effects of melting temperature and time on iron valence and crystallization of iron phosphate glasses. J. Non-Cryst. Solids. 249, 1.

Project: 81934 (Renewal of Project No. 60020)

Title: Stability of High Level Radioactive Waste Forms

PI: Dr. Theodore M. Besmann *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Allendorf, M. D. & Spear, K. E. (2000, in press). Mechanisms of silica refractory corrosion in glass-melting furnaces: Equilibrium predictions. J. Electrochem. Soc.

Besmann, T. M., Beahm, E. C., & Spear, K. E. (1999). An approach to thermochemical modeling of nuclear waste glass. Marra, J. C. & Chandler, G. T. (Eds.), Environmental Issues and Waste Management Technologies IV, 277-87. Ceramic Transactions, 93. American Ceramic Society. Westerville, OH.

Spear, K. E., Besmann, T. M., & Beahm, E. C. (1998). Thermochemical modeling of nuclear waste glass. Hou, P. Y., McNallan, M.J., Oltra, R., Opila, E. J., & Shores, D. A. (Eds.). High Temperature Corrosion and Materials Chemistry. The Electrochemical Society, 10 South Main St. Pennington, NJ. 98-9, 512-523.

Spear, K. E., Besmann, T. M., & Beahm, E. C. (1999, Apr. 11). Thermochemical modeling of glass: Application to high-level nuclear waste glass. MRS Bulletin. Germany. 24(4), 37-44.

Spear, K. E., Palmisiano, M. N., Pantano, C. G., Besmann, T. M., & Beahm, E. C. (1999). Surface modification of glass by vaporization reactions. Mountziaris, T. J., et. al. (Eds.). Proceeding Symposium Fundamental Gas-Phase and Surface Chemistry of Vapor-Phase Materials Synthesis. The Electrochemical Society, 10 South Main St. Pennington, NJ. 98-23, 388-394.

Publication Type: Presentation

Besmann, T. M., Beahm, E. C., & Spear, K. E. (1998, May 6). An approach to thermochemical modeling of high-level nuclear waste glass. 100th annual meeting of the American Ceramic Society. Cincinnati, OH.

Spear, K. E. (1998, 20 May). Thermochemical modeling applied to glass processes in industry and nuclear waste processes. Chemistry Division Seminar, NIST. Gaithersburg, MD.

Spear, K. E. (1998, Nov. 30 - Dec. 4). Thermochemical models of liquid solutions in nuclear waste glass subsystems. Materials Research Society Fall Meeting.

Spear, K. E. (1998, Oct. 15). Thermodynamic and kinetic modeling capabilities. 75 Years of Ceramics at Penn State, and the 53rd annual PCA Forum. Penn State. University Park, PA.

Spear, K. E. (1999, Apr. 25-28). Solid solution thermochemical models for phase systems in high-level nuclear waste glass. 101st annual meeting of the American Ceramic Society.

Spear, K. E. (1999, Dec. 21). A predictive thermodynamic model for glass: Applications to high-level radioactive waste. Seminar at Northeastern University (New England Local Section of ECS), Boston, MA.

Spear, K. E. (2000, Feb. 23). A predictive thermodynamic model for glass: Applications to high-level radioactive waste, corrosion in glass, furnaces, and float glass processing. Seminar at IIT (Local Section of ECS), Chicago, IL.

Spear, K. E. (2000, May 4). Theory and applications of a thermodynamic model for glass. Seminar at Georgia Tech (Local Section of ECS), Atlanta, GA.

Spear, K. E., Besmann, T. M., & Beahm, E. C. (1998, May 7). A thermochemical modeling of nuclear waste glass. Symposium on High Temperature Corrosion and Materials Chemistry. 193rd meeting of the Electrochemical Society. San Diego, CA.

Spear, K. E., Besmann, T. M., & Beahm, E. C. (1998, Jul. 22). Thermodynamic modeling of nuclear waste glass. Gordon Research Conference on High Temperature Materials Chemistry and Diagnostics. Plymouth, NH.

Spear, K. E., Besmann, T. M., & Trowbridge, L. D. (2000, Aug. 6-11). Thermochemical modeling of high-level nuclear waste glass. IUPAC-Sponsored Sixteenth International Conference on Chemical Thermodynamics (ICCT-2000), Tenth International Symposium on Thermodynamics of Nuclear Materials (STNM-2000), Hallifax, NS, Canada.

Spear, K. E., Palmisiano, M. N., Pantano, C. G., Besmann, T. M., & Beahm, E. C. (1998, Nov. 6). Surface modification of glass by vaporization reactions. Symposium on the Fundamental Gas-Phase and Surface Chemistry of Vapor-Phase Materials Synthesis. The Electrochemical Society Meeting. Boston, MA.

Publication Type: Proceeding

Besmann, T. M., Spear, K. E., & Beahm, E. C. (2000). Thermochemical models for nuclear waste glass subsystems - MgO-CaO and MgO-A12O3. Materials Research Society.

Spear, K. E. & Allendorf, M. D. (2000). Mechanisms of silica refractory corrosion in glass-melting furnaces: Equilibrium predictions. McNallan, M., Opila, E., Maruyama, T., & Narita, T. (Eds). High Temperature Corrosion and Materials Chemistry: Per Kofstad Memorial Symposium. The Electrochemical Society, Pennington, NJ. Proc. Vol. 99-38.

Spear, K. E., Besmann, T. M., & Beahm, E. C. (2000, Apr. 11). Thermochemical modeling of glass: Application to high-level nuclear waste glass. 10th International Conference on High Temperature Materials Chemistry (HTMC X). Julich, Germany.

Project: 81963 (Renewal of Project No. 65366)

Title: Physical, Chemical and Structural Evolution of Zeolite - Containing Waster Forms Produced from Metakaolinite and Calcined Sodium Bearing Waste

PI: Dr. Michael W. Grutzeck *Institution:* Pennsylvania State University

Publication Type: Proceeding

Siemer, D. D., Grutzeck, M. W., & Scheetz, B. E. (1999, Apr. 25-28). Comparison of materials for making hydroceramic waste forms. Proc. Amer. Ceram. Soc. Symposium on Waste Management Science and Technology in the Ceramic and Nuclear Industries, Indianapolis, IN. American Ceramic Society. Westerville, OH.

Separations Chemistry

Project: 54716

Title: Polyoxometalates for Radioactive Waste Treatment
PI: Dr. Michael T. Pope *Institution:* Georgetown University

Publication Type: Journal

Dickman, M. H., Gama, G. J., Kim, K. -C., & Pope, M. T. (1996). The structures of europium(III)- and uranium(IV) derivatives of [P 5 W 30 O 110] 15- . Evidence for Cryptohydration. J. Cluster Sci. 7, 67-583.

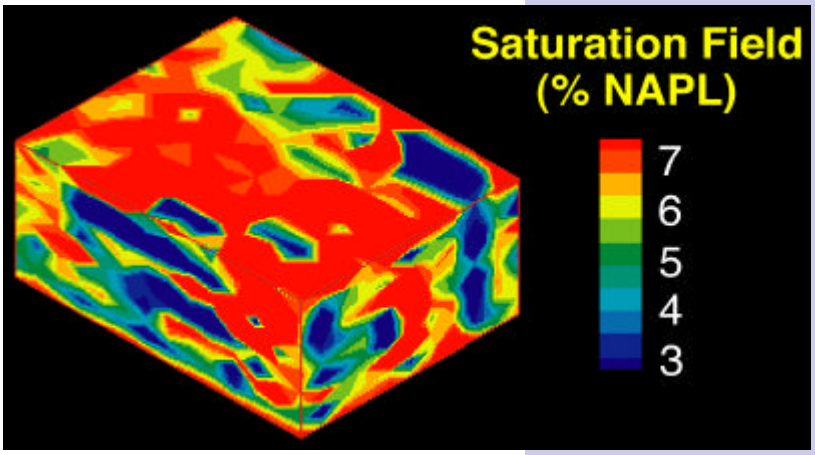
Kim, K. -C. & Pope, M. T. (1999, Sep. 22). Cation-directed structure changes in polyoxometalate chemistry. Equilibria between isomers of bis(9-tungstophosphatodioxouranate(VI)) complexes. J. Am. Chem. Soc. 121(37), 8512-8517.

Kim, K. C., et. al. (1999, Dec. 8). Slow proton exchange in aqueous solution. Consequences of protonation and hydration within the central cavity of Preyssler anion derivatives. [-M(H2 O)-GP5 W30 O110](n-). J. Am. Chem. Soc. 121(48), 11164-11170.

Müller, A., Peters, F., Pope, M. T., & Gatteschi, D. (1998). Polyoxometalates: Very large structures - nanoscale magnets. Chem. Rev. 98, 239-271.

Pope, M. T., Wei, X., Wassermann, K., & Dickman, M. H. (1998). New developments in the chemistry of heteropolytungstates of rhodium and cerium. C. R. Acad. Sci. 1. Ser. IIc, 297-304.

Wassermann, K., Dickman, M. H., & Pope, M. T. (1997). Self-assembly of supramolecular polyoxometalates. The compact, water-soluble heteropolytungstate anion [As III 12 Ce III 16 (H 2 O)36 W 148 O 524] 76ÿ. Angew. Chem. 109, 1513-1516.



NAPL saturation distribution estimated from partitioning tracer data for the Hill Air Force Base OU1 field test. [see Project #54716]

Publication Type: Patent

Pope, M. T., Creaser, I. I., & Heckel, M. C. (1997, Apr. 8). Compounds and methods for separation and molecular encapsulation of metalIons. U.S. Patent #5,618,472.

Project: 54735

Title: Development of Inorganic Ion Exchangers for Nuclear Waste Remediation
PI: Dr. Abraham Clearfield *Institution:* Texas A&M University at College Station

Publication Type: Journal

Khainakov, S. A., et. al. (1999). Hydrothermal synthesis and characterization of alkali metal titanium silicates. Journal of Materials Chem. 9, 269-272.

Pertierra, P., Salvado, M. A., Garcia-Granda, S., Bortun, A. I., & Clearfield, A. (1999). Neutron powder diffraction study of Ti2(OH)2OSiO4.1.5H2O. Inorganic Chem. 38(11), 2563-2566.

Poojary, D. M., Zhang, B., & Clearfield, A. (1998). Synthesis and structures of barium arylbisphosphonates derived from x-ray powder data. Anales de Quimica Int. Ed. 94, 401-405.

Sylvester, P. & Clearfield, A. (1999). The removal of strontium from simulated Hanford tank wastes containing complexants. Separation Science and Technology. 34(13), 2539-2551.

Sylvester, P., Clearfield, A., & Diaz, R. J. (1999). Pillared montmorillonites: cesium-selective ion-exchange materials. Science and Technology. 34(12), 2293-2305.

Trobajo, C., et. al. (1999). Hydrothermal synthesis and ion exchange properties of the novel framework sodium and potassium niobium silicates. Solvent Extraction and Ion Exchange. 17(3), 649-675.

Project: 54996

Title: Ionizing Radiation Induced Catalysis on Metal Oxide Particles
PI: Dr. Michael A. Henderson *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Alam, M., Henderson, M. A., Kaviratna, P. D., Herman, G. S., & Peden, C. H. F. (1998). Chromyl chloride chemistry at the TiO2(110) surface. J. Phys. Chem. B 102,111.

Epling, W. S., Peden, C. H. F., Henderson, M. A., & Diebold, U. (1998). Evidence for oxygen adatoms on TiO2(110) resulting from O2 dissociation at vacancy sites. Surf. Sci. 412-413, 333.

Henderson, M. A., et al. (1999). The chemistry of methanol on the TiO2(110) surface: The influence of vacancies and coabsorbed species. Faraday Discuss. 114, 313-329.

Henderson, M. A., et al. (1999, Jun. 24). Interaction of molecular oxygen with the vacuum annealed TiO2(110) surface: Molecular and dissociative channels. J. Phys. Chem. B. 103(25), 5328-5337.

Henderson, M. A., Oreto-Tapia, S., & Castro, M. E. (1998). Electron induced decomposition of CH3OH on the vacuum annealed surface of TiO2(110). Surf. Sci. 412-413, 252.

Herman, G. S., Gao, Y., Tran, T. T., & Osterwalder, J. (2000). X-ray photo-electron diffraction study of anatase thin film: TiO2(001). Surf. Sci. 447,201.

Herman, G. S., Henderson, M A., Starkweather, K. A., & McDaniel, E. P. (1999, May-Jun.). Mass- spectrometry of recoiled ions, secondary ion mass spectrometry, and Auger electron spectroscopy investigation of Y2O3-stabilized ZrO2(100) and (110). J. Vac. Sci. Technol. A. 17(3), 939-944.

Su, Y., et. al. (1998). Gamma-ray destruction of EDTA catalyzed by titania. J. Adv. Oxid. Technol. 3, 63.

Taylor, D. P., Simpson, W. C., Knutsen, K., Henderson, M. A., & Orlando, T. M. (1998). Photon stimulated desorption of cations from yttria-stabilized cubic ZrO2(100). Appl. Surf. Sci. 102, 4536.

Publication Type: Poster

Perkins, C. L. (1999). Photoconversion of adsorbed oxygen states on TiO2(110). The Sixth International Conference on the Structure of Surfaces. Vancouver, British Columbia, Canada.

Publication Type: Presentation

Henderson, M. A. (1997). Application of static secondary ion mass spectrometry in probing the interaction of water with well-defined oxide surfaces. SIMS XI, 11th International Conference on Secondary Ion Mass Spectrometry. Orlando, FL.

Henderson, M. A. (1998). Coadsorption studies with water and oxygen: A small step toward understanding the surface chemical and photochemical properties of TiO2. Invited presentation at the Department of Chemistry, University of Puerto Rico. Mayaquez, Puerto Rico.

Henderson, M. A. (1998). Coadsorption studies with water: A small step toward understanding the surface chemical and photochemical properties of TiO2. Invited presentation at the 45th National Symposium of the American Vacuum Society. Baltimore, MA.

Henderson, M. A. (1998). Ionizing radiation induced catalysis: Radiocatalytic degradation of organic contaminants in TiO2 suspensions. Invited presentation at the Notre Dame Radiation Laboratory, University of Notre Dame. South Bend, IN.

Henderson, M. A. (1998). Probing the surface chemistry of single crystal metal oxides with water. Invited presentation at the 215th National Meeting of the American Chemical Society. Dallas, TX.

Henderson, M. A. (1999). Activation of molecular oxygen on TiO2(110) by reaction with bridging hydroxyls. First International Workshop on Oxide Surfaces. Elmau, Germany.

Henderson, M. A. (1999). Electron induced decomposition of methanol on the vacuum annealed surface of TiO2(110). Environmental Molecular Sciences Symposia and First Users' Meeting. Richland, WA.

Henderson, M. A. (1999). The chemistry of methanol on the TiO2(110) surface: The influence of vacancies and coadsorbed species. Invited presentation at the 114th Faraday Discussion (The Surface Science of Metal Oxides). Ambleside, UK.

Herman, G. S. (1999). Anatase TiO2 - A structural investigation by x-ray photoelectron diffraction. The Sixth International Conference on the Structure of Surfaces. Vancouver, B. C.

Herman, G. S. (1999). Characterization of oxide surfaces by mass-spectroscopy of recoiled ions. Surface Analysis '99, Applied Surface Symposium, American Vacuum Society. Waukesha, WI.

Peden, C. H. F. (1997, Sept.). The growth, structure, and surface chemistry of oxide films as model surfaces. Invited presentation at the 17th National Congress of the Mexican Surface Science and Vacuum Society. Mazatlan, Mexico.

Peden, C. H. F. (1998, Apr.). Water adsorption and reaction as a probe of oxide surface structure and chemistry. Invited presentation for the Department of Chemistry, Texas A&M University. College Station, TX.

Perkins, C. L. (1999). Interactions of oxygen, water, and defects on the TiO2(110) surface. Invited presentation at the University of Illinois/Chicago Chemistry Department Seminar. Chicago, IL.

Perkins, C. L. (1999). Photoconversion of adsorbed oxygen states on TiO2(110). 46th International Symposium of the American Vacuum Society. Seattle, WA.

Perkins, C. L. (1999). Surface chemistries of group IV oxides and borides. Invited presentation at the Washington State University seminar. Richland, WA.

Su, Y. (1997). Radiocatalytic degradation of organic contaminants in colloidal TiO2 and ZrO2 suspensions. The Third International Conference on TiO2 Photocatalytic Purification and Treatment of Water and Air. Orlando, FL.

Su, Y. (1999). Radiocatalytic and photocatalytic studies of oxidation of organics and reduction of water. The 195th Meeting of the Electrochemical Society. Seattle, WA.

Su, Y. (1999). Radiocatalytic degradation of organic contaminants in TiO2 suspensions. 214th National Meeting of the American Chemical Society. Las Vegas, NV.

Su, Y. (1999, May 2-6). Radiocatalytic and photocatalytic studies of oxidation of organics and reduction of water. The 195th Meeting of the Electrochemical Society, Seattle, WA.

Su, Y. (1999, May 24-28). Radiocatalytic and photocatalytic studies of metal ion reduction and water cleavage into hydrogen. The 5th International Conference on Advanced Oxidation Technologies for Water and Air Remediation, Albuquerque, NM.

Project: 59990

Title: Fundamental Chemistry, Characterization, and Separation of Technetium Complexes in Hanford Waste

PI: Dr. Norman C. Schroeder *Institution:* Los Alamos National Laboratory

Publication Type: Journal

Schroeder, N. C., Ball, J. R., Radzinski, S. D., Whitener, G. D., & Ashley, K. R. (1999). Reillex(TM)-HPQ anion exchange column chromatography: Removal of Pertechnetate from DSSF-5 simulant at various flow rates. Solvent Extr. Ion Exc. 17(6), 1543-1556.

Publication Type: Other

Schroeder, N. C., Radzinski, S. D., Ashley, K. R., Truong, A. P., & Szczepaniak, P. A. (1998). Technetium oxidation state adjustment for hanford waste processing. Lombardo, N. J. & Schulz, W. W. (Eds.),

Science and Technology for Disposal of Radioactive Tank Waste. Plenum Publishing Corporation. New York, NY.

Publication Type: Proceeding

Ashley, K. R., Whitener, G. D., Schroeder, N. C., Ball, J. R., & Radzinski, S. D. (1999). Bond, A. H., Dietz, M. L. & Rogers, R. D. (Eds.), Progress in Metal Ion Separation and Preconcentration, ACS Symposium Series 716, American Chemical Society. Washington, D. C. 219.

Project: 60017

Title: Removal of Technetium, Carbon Tetrachloride, and Metals from DOE Properties

PI: Dr. Thomas E. Mallouk *Institution:* Pennsylvania State University

Publication Type: Journal

Ponder, S. M. & Mallouk, T. E. (1999, Oct.). Recovery of ammonium and cesium ions from aqueous waste streams by sodium tetraphenylborate. Ind. Eng. Chem. Res. 38(10), 4007-4010.

Publication Type: Presentation

Ponder, S. M., et. al. (1999, Aug. 22). Ferragels: Supported zero-valent iron as a remediant for aqueous metal ion wastes. Abstr. Pap. Am. Chem. S. 218, U1089-U1089, Part 1.

Publication Type: Proceeding

Ponder, S. M., Ford, J. R., Darab, J. G., & Mallouk, T. E. (1999, in press). Ferragels: A new family of materials for remediation of aqueous metal ion solutions. MRS Symp. Proceedings.

Project: 60123

Title: Potential-Modulated Intercalation of Alkali Cations into Metal Hexacyanoferrate Coated Electrodes

PI: Dr. Daniel T. Schwartz *Institution:* University of Washington

Publication Type: Journal

Haight, S. M., Schwartz, D. T., & Lilga, M. A. (1999). In-situ oxidation state profiling of nickel hexacyanoferrate derivatized electrodes using line-imaging Raman spectroscopy and multivariate calibration. J. Electrochem. Soc. 146, 1866.

Project: 60313

Title: Radiation Effects on Transport and Bubble Formation in Silicate Glasses

PI: Dr. Alexander D. Trifunac *Institution:* Argonne National Laboratory

Publication Type: Journal

Shkrob, I. A., Tadjikov, B. M., & Trifunac, A. D. (2000, Feb.). Magnetic resonance studies on radiation-induced point defects in mixed oxide glasses. I. Spin centers in B2O3 and alkali borate glasses. J. Non-Cryst. Solids. 262(1-3), 6-34.

Shkrob, I. A., Tadjikov, B. M., & Trifunac, A. D. (2000, Mar.). Magnetic resonance studies on radiation-induced point defects in mixed oxide glasses. II. Spin centers in alkali silicate glasses. J. Non-Cryst. Solids. 262(1-3), 35-65.

Shkrob, I. A., Tadjikov, B. M., Chemerisov, S. D. & Trifunac, A. D. (1999, Sep. 15). Electron trapping and hydrogen atoms in oxide glasses. J. Chem. Phys. 111(11), 5124-5140.

Project: 73803 (Renewal of Project No. 55087)

Title: Next Generation Extractants for Cesium Separation from High-Level Waste: From Fundamental Concepts to Site Implementation

PI: Dr. Bruce A. Moyer *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Bond, A. H., Dietz, M. L., & Chiarizia, R. (2000, in press). Incorporating size-selectivity into synergistic solvent extraction: A review of crown ether-containing systems. Ind. Eng. Chem. Res.

Bond, A. H., et. al. (1999). Synergistic solvent extraction of alkaline Earth cations by mixtures of Di-n-octylphosphoric acid and stereoisomers of Dicyclohexano-18-crown-6. Anal. Chem. 71, 2757-2765.

Bryan, J. C., et. al. (1999). Cesium recognition by supramolecular assemblies of 2-Benzylphenol and 2-Benzylphenolate. Structural Chem. 10(3), 187-203.

Chiarizia, R., et. al. (1999, Aug. 22). Synergistic effects in the extraction of metal ions by mixtures of dialkylphosphoric acids and crown ethers. Abstr. Pap. Am. Chem. S. 218, U1049-U1049, Part 1.

Chiarizia, R., Urban, V., Thiyagarajan, P., Bond, A. H., & Dietz, M. L. (2000). Small angle neutron scattering investigation of the species formed in the extraction of Sr(II) by mixtures of Di-n-octylphosphoric acid and dicyclohexano-18-crown-6. Solvent Extr. Ion Exch. 18, 451-478.

Dietz, M. L., et. al. (1999). Comparison of column chromatographic and precipitation methods for the purification of a macrocyclic polyether extractant. Sep. Sci. Technol. 34, 2943-2956.

Dietz, M. L., et. al. (1999). Ligand reorganization energies as the basis for the design of synergistic metal ion extractants. J. Chem. Soc., Chem. Commun. 1177-1178.

Haverlock, T. J., Bonnesen, P. V., Sachleben, R. A., & Moyer, B. A. (2000). Analysis of equilibria in the extraction of cesium nitrate by calix[4]arene-bis(t-octylbenzo-crown-6) in 1,2-dichloroethane. J. Incl. Phenom. Mol. Recognit. Chem. 36(1), 21-37.

Hay, B. P. & Nicholas, J. B. (2000, in press). Unexpected binding modes in tetramethoxycalix(4)arene: Implications for ligand design. J. Am. Chem. Soc.

Nicholas, J. B. & Hay, B. P. (1999, Dec. 2). Anisole as an ambidentate ligand: Ab initio molecular orbital study of alkali metal cations binding to anisole. J. Phys. Chem. A. 100(48), 9815-9820.

Nicholas, J. B., Dixon, D. A., & Hay, B. P. (1999). Ab initio molecular orbital study of cation-¼ binding between the alkali metal cations and Benzene. J. Phys. Chem. 103, 1394-1400.

Sachleben, R. A., et. al. (1999). Dideoxygenated calix[4]rene crown-6 ethers prefer the 1,3-alternate conformation and exhibit enhanced selectivity for cesium over potassium and rubidium. J. Chem. Soc., Chem. Commun. 1751-1752.

Sachleben, R. A., et. al. (1999). Surveying the extraction of cesium nitrate by 1,3-alternate calix[4]-arene crown-6 ethers in 1,2-dichloroethane. Solvent Extr. Ion Exch. 17(6), 1445-1459.

Publication Type: Media report

Moyer, B. A., et. al. (2000, Feb.). Highlights of technology developed in the chemical separations group. Highlight released to Chemical Engineering Magazine. Joint sponsorship of the Efficient Separations and Processing Cross-cutting Program (EW4030000), Environmental Management Science Program (EW4090100), and the Office of Basic Energy Sciences (KC0302020), U. S. Department of Energy.

Publication Type: Presentation

Bond, A. H., Dietz, M. L., Chiarizia, R., & Hay, B. P. (2000, Mar. 26-30). Synergistic extraction of mono-, di-, and trivalent cations by dicyclohexano-18-crown-6 and dialkylphosphoric acids. 219th American Chemical Society National Meeting, San Francisco, CA.

Bond, A. H., Dietz, M. L., Chiarizia, R., Herlinger, A. W., & Hay, B. P. (1999, Aug. 22). Influence of diluent solvation properties on synergistic solvent extraction by dialkylphosphoric acids and dicyclohexano-18-crown-6. 218th American Chemical Society Meeting. New Orleans, LA.

Bond, A. H., et. al. (1998, Aug. 23-27). Synergistic extraction of cations by dicyclohexano-18-crown-6 and dialkyl phosphoric acids in an alcohol diluent. 216th American Chemical Society Meeting. Boston, MA.

Chiarizia, R., Dietz, M. L., Bond, A. H., Hay, B. P., & Moyer, B. A. (1999, Jul. 11). Synergism in the extraction of metal ions by mixtures of organophosphorous acids and substituted crown ethers. International Solvent Extraction Conference (ISEC ’99). Barcelona, Spain.

Chiarizia, R., Urban, V., Thiyagarajan, P., Bond, A. H., & Dietz, M. L. (2000, Mar. 26-30). SANS investigations of organic-phase speciation in the extraction of Sr(II) by mixtures of di-n-octylphosphoric acid and dicyclohexano-18-crown-6. 219th American Chemical Society National Meeting, San Francisco, CA.

Delmau, L., Bryan, J. C., Sachleben, R. A., Hay, B. P., & Moyer, B. A. (1999, Mar. 21). Benzyl phenol derivatives: Building blocks for calixarenes. I&EC Symposium on Calixarene Molecules for Separations. 217th American Chemical Society Meeting. Anaheim, CA. Joint sponsorship with the Office of Basic Energy Sciences (KC0302020), U. S. Department of Energy.

Dietz, M. L., Bond, A. H., Chiarizia, R., Huber, V. J., Herlinger, A. W., & Hay, B. P. (1999, Aug. 22-26). Synergistic effects in the extraction of metal ions by mixtures of dialkylphosphoric acids and crown ethers. 218th American Chemical Society Meeting. New Orleans, LA.

Dietz, M. L., et. al. (1998, Apr. 2). Synergism in the extraction of cations by mixtures of dialkylphosphoric acids and substituted crown ethers. Abstr. Pap. Am. Chem. S. 215, U666-U667, Part 1.

Dietz, M. L., et. al. (2000, Mar. 26-30). Ligand reorganization energies as a basis for the design of metal ion extraction systems. Invited presentation at the 219th American Chemical Society National Meeting, San Francisco, CA.

Haverlock, T. J., Bonnesen, P. V., Sachleben, R. A., & Moyer, B. A. (1999, Oct. 18-21). The relationship between species and selectivity in the extraction of cesium and potassium nitrate by calix[4]arene-bis(t-octylbenzo-crown-6) in 1,2-dichloroethane. Eleventh Symposium on Separation Science and Technology for Energy Applications. Gatlinburg, TN.

Haverlock, T. J., Bonnesen, P. V., Sachleben, R. A., & Moyer, B. A. (1997, Sept. 7-11). Cs/K selectivity of a lipophilic calix[4]arene-crown-6 extractant in liquid-liquid separations from nitrate media. 214th American Chemical Society National Meeting. Las Vegas, NV.

Hay, B. P. & Nicholas, J. B. (1999, Jul. 22). Calixarene complexes with alkali cations: There is more to binding than you realized. Environmental Molecular Sciences Symposia and First EMSL Users' Meeting. Pacific Northwest National Laboratory. Richland, WA.

Hay, B. P. & Nicholas, J. B. (1999, Mar. 21). Calixarene complexes with alkali cations: There is more to binding than you realized. Invited presentation at the I&EC Symposium on Calixarene Molecules for Separations, 217th American Chemical Society Meeting. Anaheim, CA.

Hay, B. P. (1998, Oct. 20-22). Ligand design with molecular mechanics. INEEL Science Integrated Workshop, Environmental Management Science Program, Idaho Falls, ID.

Hay, B. P., Dietz, M. L., & Horwitz, E. P. (2000, Mar. 26-30). Optimization of the SREX reagent using a molecular mechanics model. Invited presentation at the 219th American Chemical Society National Meeting, San Francisco, CA.

Huber, V. J., Bond, A. H., Chiarizia, R., & Dietz, M. L. (1998, Aug. 23-27). An improved synthesis of individual dicyclohexano crown isomers. 216th American Chemical Society National Meeting. Boston, MA.

Moyer, B. A. (1999, Aug. 22-24). Chemical principles and their use toward remediation of radioactive contamination in wastes and the environment. 218th American Chemical Society National Meeting. New Orleans, LA. Joint sponsorship of the Efficient Separations and Processing Cross-cutting Program (EW4030000), Environmental Management Science Program (EW4510000), and the Office of Basic Energy Sciences (KC302020), U. S. Department of Energy.

Moyer, B. A. (1999, Dec. 4). Crown ethers for selective extraction of metal ions: From fundamental to applied chemistry. Invited presentation at Kyoto University, Kyoto, Japan. Joint sponsorship of the Efficient Separations and Processing Cross-cutting Program (EW4030000), Environmental Management Science Program (EW4090100), and the Office of Basic Energy Sciences (KC0302020), U. S. Department of Energy.

Moyer, B. A. (1999, Nov. 12). An overview of the R&D in separation science and technology in the USA and future trends: Environmental and waste problems of the USDOE. Invited presentation at Japan Atomic Energy Research Institute (JAERI), Tokai-mura, Ibaraki, Japan. Joint sponsorship of the Efficient Separations and Processing Cross-cutting Program (EW4030000), Environmental Management Science Program (EW4090100), and the Office of Basic Energy Sciences (KC0302020), U. S. Department of Energy.

Moyer, B. A. (1999, Nov. 15). Selective extraction of metal ions by crown ethers: Principles and Applications. National Institute for Resources and Environment, Tsubuka, Ibaraki, Japan. Joint sponsorship of the Efficient Separations and Processing Cross-cutting Program (EW4030000), Environmental Management Science Program (EW4090100), and the Office of Basic Energy Sciences (KC0302020), U. S. Department of Energy.

Moyer, B. A. (1999, Nov. 17). New separation technologies for rad-waste management: Metal separation processes developed at ORNL. Invited presentation at Japan Atomic Energy Research Institute (JAERI), Tokai-mura, Ibaraki, Japan. Joint sponsorship of the Efficient Separations and Processing Cross-cutting Program (EW4030000), Environmental Management Science Program (EW4090100), and the Office of Basic Energy Sciences (KC0302020), U. S. Department of Energy.

Moyer, B. A. (1999, Nov. 19). Principles and applications of crown ethers for selective extraction of metals from wastes. Invited presentation at Himeji Institute of Technology, Himeji, Japan. Joint sponsorship of the Efficient Separations and Processing Cross-cutting Program (EW4030000), Environmental Management Science Program (EW4090100), and the Office of Basic Energy Sciences (KC0302020), U. S. Department of Energy.

Moyer, B. A., Bonnesen, P. V., Delmau, L. H., Haverlock, T. J., & Sachleben, R. A. (1998, Sep. 9). Development of an alkaline-side Cs SX process applicable to Savannah River HLW using a calixarene-crown extractant: Interim progress. Solvent Extraction Working Group Meeting for Savannah River HLW, Argonne National Laboratory. Joint sponsorship with the Efficient Separations and Processing Crosscutting Program (EW4030000) and Westinghouse Savannah River Company.

Moyer, B. A., et. al. (1997, Oct. 15-17). Crown compounds as separation agents for environmental remediation from basic concepts to applications. Symposium on Molecular Sciences for the Environment, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory. Joint sponsorship with the Efficient Separations and Processing Cross-cutting Program (EW4030000) and the Office of Basic Energy Sciences (KC0302020), U. S. Department of Energy.

Moyer, B. A., et. al. (1998, Jul. 27-30). Design and synthesis of the next generation of crown ethers for waste separations. DOE EMSP Scientific Workshop. Chicago, IL.

Moyer, B. A., et. al. (1999, Mar. 21-26). Alkaline-side CSEX process for Savannah River high-level waste. 217th American Chemical Society National Meeting. Anaheim, CA. Joint sponsorship with the Efficient Separations and Processing Crosscutting Program, Office of Science and Technology, Ofiice of Environmental Management, U. S. Department of Energy.

Moyer, B. A., et. al. (2000, Jan. 26). Solvent extraction of fission products from alkaline nuclear waste. Invited presentation at Syracuse University, Syracuse, NY. Joint sponsorship of the Efficient Separations and Processing Cross-cutting Program (EW4030000), Environmental Management Science Program (EW4090100), and the Office of Basic Energy Sciences (KC0302020), U. S. Department of Energy.

Moyer, B. A., et. al. (2000, Mar. 26-31). Approaches to the remediation of alkaline high-level waste using solvent extraction. 219th National Meeting of the American Chemical Society, San Francisco, CA.

Moyer, B. A., et. al. (2000, Mar. 3). Fundamental research toward a process for nuclear-waste treatment: Cesium separation using calix-crown ethers. Invited presentation for the Department of Chemistry, Virginia Polytechnic Institute & State University, Blacksburg, VA. Joint sponsorship of the Efficient Separations and Processing Cross-cutting Program (EW4030000), Environmental Management Science Program (EW4090100), and the Office of Basic Energy Sciences (KC0302020), U. S. Department of Energy.

Moyer, B. A., Sachleben, R. A., & Alexandratos, S. D. (1999, Apr. 27-29). Ion exchange approach to the removal of ionic contaminants from groundwater. US DOE Subsurface Contamination Focus Area Mid-Year Review Meeting. Augusta, GA.

Moyer, B. A., Sachleben, R. A., Haverlock, T. J., & Alexandratos, S. D. (1999, Sept. 22). Ion exchange approach to the removal of ionic contaminants from groundwater. US DOE Oak Ridge Operations Environmental Management Science Program Workshop. Oak Ridge, TN.

Nicholas, J. B. & Hay, B. P. (1998, Jun. 17). A theoretical study of alkali cation complexes with tetramethoxycalix[4]arene. Northwest Regional American Chemical Society Meeting. Richland, WA.

Nicholas, J. B. & Hay, B. P. (1998, Jun. 6). A theoretical study of alkali cation complexes with tetramethoxycalix[4]arene. XXIII International Symposium on Macrocyclic Chemistry. Turtle Bay, Oahu, Hawaii.

Sachleben, R. A., et. al. (1999, Aug. 22-24). Calix[4]arene crown-6 ethers recent developments in enhanced cesium-selective extractants. 218th American Chemical Society National Meeting. New Orleans, LA.

Sachleben, R. A., et. al. (1999, Aug. 6). Recent developments in enhanced cesium-selective extractants calix[4]arene crown-6 ethers. DuPont Pharmaceuticals. N. Billerica, MA.

Sachleben, R. A., et. al. (1999, Mar. 21-26). Optimizing cesium-selective extraction by calix[4]arene crown ethers through ligand design. 217th American Chemical Society National Meeting. Anaheim, CA.

Sachleben, R. A., et. al. (1999, Sep. 19-23). Making the best even better enhancing the cesium selectivity of calixarene crown ethers through ligand design. Fifth International Conference on Calixarene Chemistry. Perth, Australia.

Yang, L., Dixon, D. A., & Hay, B. P. (1997, Jun. 6). MM3 calculations on alkali cation benzene complexes. International Conference on Structural and Mechanistic Organic Chemistry. Athens, GA.

Yang, L., Dixon, D. A., & Hay, B. P. (1997, Sep. 8). Molecular mechanics (MM3) calculations on calixarene complexes with alkali metal cations. The Importance of _-Cation Interactions. Inorganic Poster Session. 214th American Chemical Society Meeting. Las Vegas, NV.

Publication Type: Proceeding

Bond, A. H., Dietz, M. L., Huber, V. J., Herlinger, A. W., & Hay, B. P. (1999, Mar. 21). Diluent effects in synergistic solvent extraction by dicyclohexano-18-crown-6 and dialkylphosphoric acids. Abstr. Pap. Am. Chem. S. 217, U880-U880, Part 1.

Chiarizia, R., et. al. (1999, Jul. 11-16, in press). Synergistic effects in the extraction of metal ions by mixtures of dialkylphosphoric acids and substituted crown ethers. Proceedings of the International Solvent Extraction Conference, Barcelona, Spain.

Delmau, L. H., et. al. (2000). Benzyl phenol derivatives: Extraction properties of calixarene fragments. Lumetta, G. J., Rogers, R. D., & Gopalan, A. S. (Eds.). Calixarene Molecules for Separations. ACS Symposium Series, American Chemical Society, Washington, D. C. 757, 86-106.

Hay, B. P. (1999). A molecular mechanics method for predicting the influence of ligand structure on metal ion binding affinity. Bond, A. H., Dietz, M. L., & Rogers, R. D. (Eds.). Metal Ion Separation and Preconcentration: Progress and Opportunities. ACS Symposium Series 716, American Chemical Society, Washington, DC. 102-113.

Publication Type: Theses/Dissertations

Stine, C. L. (2000). Design and synthesis of the next generation of crown ethers for waste separations. Ph. D. dissertation, University of Tennessee, Knoxville, TN.

Project: 73824 (Renewal of Project No. 59982)

Title: Reactivity of Peroxynitrite: Implications for Hanford Waste Management and Remediation

PI: Dr. Sergei V. Lymar *Institution:* Brookhaven National Laboratory

Publication Type: Journal

Coddington, J. W., Hurst, J. K., & Lymar, S. V. (1999). Hydroxyl radical formation during peroxynitrous acid decomposition. J. Am. Chem. Soc. 121, 2438-2443.

Coddington, J. W., Wherland, S., & Hurst J. K. (1999). Radical intermediates in peroxynitrite reactions. Nitric Oxide. 3, 37.

Czapski, G., Lymar, S. V., & Schwarz, H. A. (1999). Acidity of the carbonate radical. J. Phys. Chem. A. 103, 3447-3450.

Gerasimov, O. V. & Lymar, S. V. (1999). Pathways of decomposition and one-electron oxidation by peroxynitrous acid. Nitric Oxide. 3, 7.

Gerasimov, O. V. & Lymar, S. V. (1999, Sep. 20). The yield of hydroxyl radical from the decomposition of peroxynitrous acid. Inorg. Chem. 38(19), 4317-4321.

Goldstein, S., Saha, A., Lymar, S. V., & Czapski, G. (1998). Oxidation of peroxynitrite by inorganic radicals: A pulse radiolysis study. J. Am. Chem. Soc. 120, 5549-5554.

Lymar, S. V. & Hurst, J. K. (1998). ACO 2 -catalyzed one-electron oxidations by peroxynitrite: Properties of the reactive intermediate. Inorganic Chemistry. 37, 294-301.

Lymar, S. V. & Hurst, J. K. (1998). Radical nature of peroxynitrite reactivity. Chem. Res.Toxicol. 11, 714-715.

Project: 74019 (Renewal of Project No. 54864)

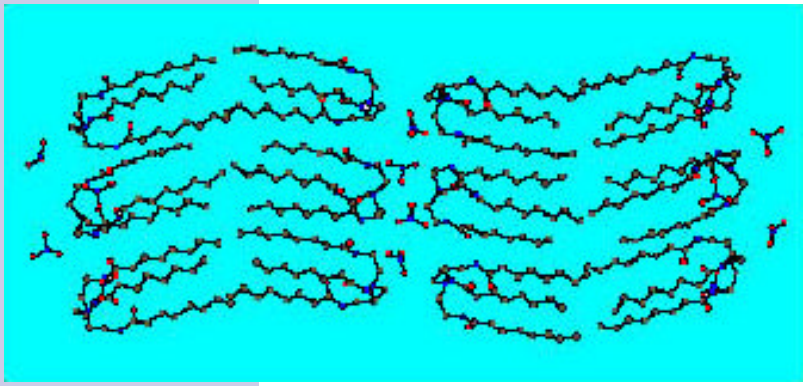
Title: Supramolecular Chemistry of Selective Anion Recognition for Anions of Environmental Relevance

PI: Dr. Kristin Bowman-James *Institution:* University of Kansas

Publication Type: Journal

Aguilar, J. A., et. al. (2000, in press). Fluoride ion receptors: A comparison of a polyammonium monocycle versus its bicyclic corollary. Supramolec. Chem.

Clifford, T., Mason, S., Llinares, J. M., & Bowman-James, K. (2000). Snapshots of fluoride binding in an Azacryptand. J. Am. Chem. Soc. 122, 1814-1815.

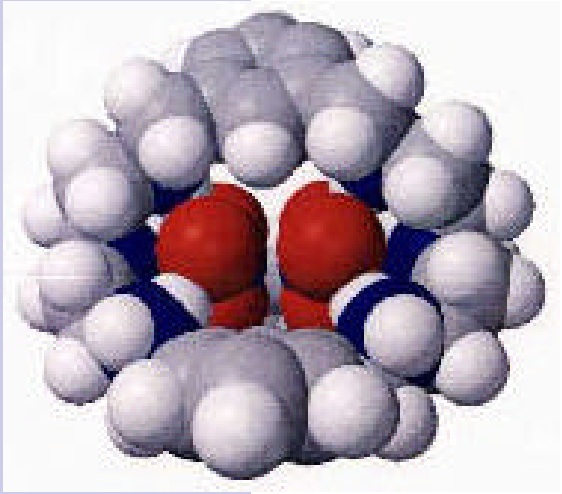


Contaminant Binding Science - The crystal structure of one of a tripodallipophilic adide with nitrate ion, illustrated above, was developed for a University of Kansas project, which uses a combination of anion and catioin complexing agents to extract cesium nitrate. [see Project #74019, renewal of #54864]

Danby, A., Seib, L., Alcock, N. W., & Bowman-James, K. (2000). Novel structural determination of a bilayer network formed by a tripodal lipophilic amide in the presence of anions. Chem. Commun. 39, 1371-1375.

Gerasimchuk, O. A., et. al. (2000, Apr. 3). Binding of phosphate with a simple hexaaza polyammonium macrocycle. Inorg. Chem. 39(7), 1371-1375.

Hossain, M. A., Llinares, J. M., Powell, D., & Bowman-James, K. (2001, in press). Multiple hydrogen bond stabilization of a sandwich complex of sulfate between two macrocyclic tetraamides. Inorg. Chem.



Nitrate inclusion complex with a polyammonium receptor. [see Project #74019, renewal of #54864]

Kavallieratos, K., et. al. (2000). Tris(2-aminoethyl)amine (tren) triamide derivatives enhance CsNO3 extraction in 1,2-dichloroethane via a dual-host strategy. Anal. Chem. 72, 5258-6264.

Mason, S., Clifford, T., Seib, L., Kuczera, K., & Bowman-James, K. (1998). Unusual encapsulation of two nitrates in a single bicyclic cage. J. Am. Chem. Soc. 120, 8899-8900.

Qian, Q., Wilson, G. S., Bowman-James, K., & Girault, H. H. (2001). Microities detection of NO3- by facilitated k+ transfer. Anal. Chem. 73, 497-503.

Wiórkiewicz-Kuczera, et. al. (1999). Solid state to solution: Crystal structure and molecular dynamics simulations of a polyammonium nitrate host, New J. Chem. 23, 1007-1013.

Publication Type: Other

Bianchi, A., Bowman-James, K., & García-Espana, E. (Eds.). (1997), Supramolecular Chemistry of Anions, Wiley-VCH. New York, NY. 461.

Wiórkiewicz-Kuczera, J. & Bowman-James, K. (1997). Anion Binding Receptors: Theoretical Studies. Bianchi, A., Bowman-James, K., & García-España, E. (Eds.), Supramolecular Chemistry of Anions. Wiley-VCH, New York, NY. 335-354.

Publication Type: Paper

Bowman-James, K. & Mason, S. (1998, Aug.). Supramolecular chemistry of anions. 216th National Meeting of the American Chemical Society, Boston, MA.

Bowman-James, K. (1999, Jul. 18-23). Supramolecular chemistry of anions and macrocycles. Plenary Lecture at the XXIV International Symposium on Macrocyclic Chemistry, Bellaterra (Barcelona), Spain.

Bowman-James, K. (2000, Jul. 2-7). Exploration in anion coordination chemistry. Symposium Lecture at the XXV International Symposium on Macrocyclic Chemistry, Saint Andrews, Scotland.

Kavallieratos, K., et. al. (1999, Mar.). New anion receptors and their role in solvent extraction. 217th National Meeting of the American Chemical Society, Anaheim, CA.

Publication Type: Press release

Moyer, B. A. (1998, Sep. 7). Two nitrates in a cage. C&E News concentrate. 30.

Project: 81883

Title: Mechanisms and Kinetics of Organic Aging and Characterization of Intermediates in High-Level Waste

PI: Dr. Donald M. Camaioni *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Cook, A. R., et. al. (2001, in press). Reducing radicals in nitrate solutions. The NO3 system revisited. J. Phys. Chem. A.

Fessenden, R. D., Meisel, D., & Camaioni, D. M. (2000). Addition of oxide radical ions (O) to nitrite and oxide ions (O2) to nitrogen dioxide. J. Am. Chem. Soc. 122, 3773-3774.

Publication Type: Poster

Camaioni, D. M., Dupuis, M., & Franz, J. A. (2000, Jun. 29). Theoretical characterization of organic radicals in solution. Gomberg 2000 (8th International Symposium on Organic Free Radicals). Ann Arbor, MI.

Publication Type: Presentation

Autrey, S. T. (1999, Apr. 30). Nitrosyl transfer reactions are not catalyzed by Al(OH)4. Notre Dame Radiation Laboratory and Pacific Northwest National Laboratory EEMSP Coordination Meeting and Technical exchange. Notre Dame, IN.

Camaioni, D. M. (1998, Nov. 17). Mechanisms and kinetics of organic aging in high level wastes. EMSP/Tanks Focus Area Workshop. Richland, WA.

Camaioni, D. M. (1998, Oct. 29). Mechanisms and kinetics of the degradation of organic complexants in nuclear waste. Chemistry Seminar, Notre Dame Radiation Laboratory. Notre Dame, IN.

Camaioni, D. M. (1999, Aug. 22-26). Thermochemical kinetic analysis of thermal pathways for oxidation of organic complexants in high level wastes. First Accomplishments of the Environmental Management Science Program. Annual Meeting of the American Chemical Society. New Orleans, LA.

Camaioni, D. M., Orlando, T. M., & Meisel, D. (2000, Apr. 25-27). Radiolytic and thermal processes in homogenous and heterogenous high level waste. EMSP National Workshop. Atlanta, GA.

Dupuis, M. (1999, Aug.). Electronic structure and reactivity in the condensed phase. Physical Chemistry Colloquium. Department of Chemistry. University of Notre Dame. South Bend, IN.

Dupuis, M. (1999, Nov.). Theoretical characterization of electronic structure and reactivity in the condensed phase. Department of Chemistry. University of Alberta. Edmonton, Alberta, Canada.

Dupuis, M. (2000, Mar.). Electronic structure and reactivity in the condensed phase: Computational studies. Physical Chemistry Seminar. Department of Chemistry. University of Washington. Seattle, WA.

Dupuis, M. (2001, Oct.). Recent research on electronic structure and reactivity in the aqueous phase. University of Tokyo. Tokyo, Japan.

Dupuis, M. (2001, Oct.). Recent research on electronic structure and reactivity in the aqueous phase. University of Kyoto. Kyoto, Japan.

Publication Type: Proceeding

Babad, H. & Camaioni, D. M. (2000, Feb. 27 - Mar. 2). The aging of organic chemicals in Hanford high-level wastes. Proceedings of the Waste Management 2000 Conference. Tucson, AZ.

Camaioni, D. M. & Autrey, S. T. (2000). Thermochemical kinetic analysis of mechanism for thermal oxidation of organic complexants in high level waste. In Eller, P. G. & Heineman, W. R. (Eds.). Nuclear Site Remediation on First Accomplishments of the Environmental Management Program. ACS Symposium Ser. 778. American Chemical Society. Washington, D. C. 21, 342-361.

Dupuis, M. (2000, Mar.). Electronic structure and reactivity in the condensed phase: Computational studies. Symposium on "Potential Energy Surfaces: From Polyatomics to Macromolecules." 219th American Chemical Society National Meeting. San Francisco, CA.

Meisel, D., Camaioni, D. M., & Orlando, T. M. (2000). Radiation and chemistry in nuclear waste: The NOx system and organic aging. In Eller, P. G. & Heineman, W. R. (Eds.). Nuclear Site Remediation on First Accomplishments of the Environmental Management Program. ACS Symposium Ser. 778. American Chemical Society. Washington, D. C. 21, 342-361.

Project: 81912 (Renewal of Project No. 65409)

Title: Electroactive Materials for Anion Separation – Technetium from Nitrate

PI: Timothy L. Hubler *Institution:* Pacific Northwest National Laboratory

Publication Type: Presentation

Gronda, A. M. & Smyrl, W. H. (1999, Oct. 17-22). High capacity electroactive polymers for radioactive waste removal. Abstract at the 196th Electrochemical Society Meeting. Honolulu, HI.

Hubler, T. L., Anderson, G. M., Sukamto, J. H., Lilga, M. A., & Rassat, S. D. (1999, Aug. 22). Polyvinylferrocene (PVF) polymers as electroactive ion-exchange materials for separation of pertechnetate ion from high nitrate ion containing wastes: Issues and synthetic strategies. Abstr. Pap. Am. Chem. S. 218, U1050-U1050, Part 1.

MIXED WASTE

Analytical Chemistry & Instrumentation

Project: 54751

Title: High Fluence Neutron Source for Nondestructive Characterization of Nuclear Waste

PI: Dr. Mark M. Pickrell *Institution:* Los Alamos National Laboratory

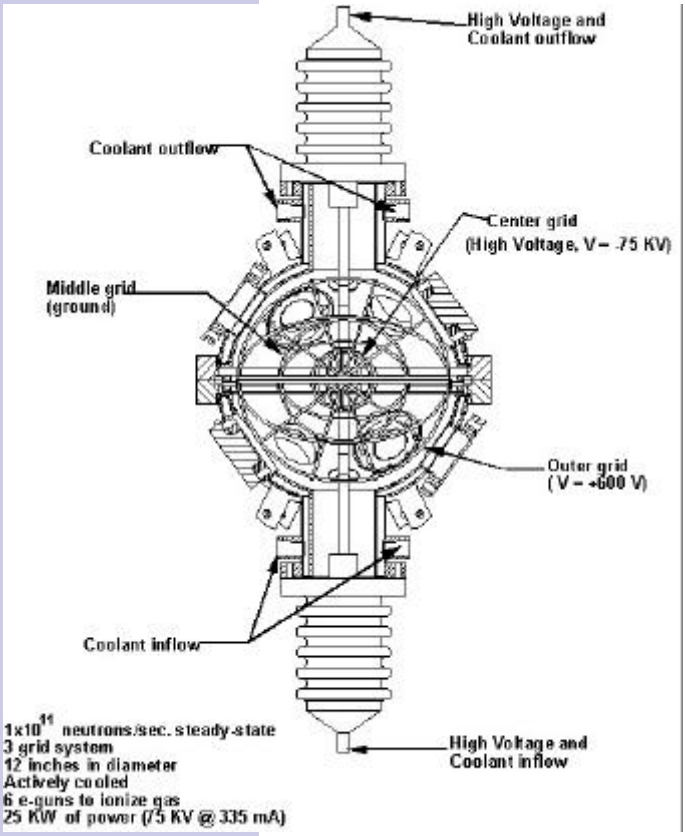
Publication Type: Journal

Barnes, D. C. & Nebel, R. A. (1998). Stable, thermal equilibrium. Large-amplitude, spherical plasma oscillations in electrostatic confinement devices. Physics of Plasmas, 5, 2498.

Nebel, R. A. & Barnes, D. C. (1998). The periodically oscillating plasma sphere. Fusion Tech. 38, 28.

Publication Type: Presentation

Nebel, R. A. & Barnes, D. C. (1997, Apr.). The periodically oscillating plasma sphere. Paper 1B-3 presented at the 1997 Sherwood Theory Meeting, Madison, WI.



Cutaway schematic of the Intense Neutron Source (INS). This source is to be used for assay applications, primarily for TRU waste. Its intensity should allow for real-time assay. [see Project #54751]

Nebel, R. A., Cole, A. J., & Umstadter, K. R. (1999, Oct.). The intense neutron source. Presentation at the 18th IEEE Symposium on Fusion Engineering, Albuquerque, NM.

Nebel, R. A., et. al. (1997). The Los Alamos intense neutron source. Winter ANS meeting, Albuquerque, NM.

Nebel, R. A., et. al. (1998). Innovative energy sources and advanced applications: The Los Alamos intense neutron source. Presentation at ECOMAP98, Kyoto, Japan.

Publication Type: Proceeding

Barnes, D. C., Nebel, R. A., Schauer, M. M., & Pickrell, M. M. (1997, May 19-21). Inertial electro-magnetostatic plasma neutron sources. Paper 7EO4, 1997 IEEE International Conference on Plasma Science, San Diego, CA. 319.

Nebel, R. A., et. al. (1997, Mar.). The Los Alamos intense neutron source. Proceedings of the 2nd Symposium on Current Trends in International Fusion Research: Review and Assessment. Washington, D. C.

Project: 55146

Title: Adsorption/Membrane Filtration as a Contaminant Concentration and Separation Process for Mixed Wastes and Tank Wastes

PI: Dr. Mark M. Benjamin *Institution:* University of Washington

Publication Type: Journal

Green-Pedersen, H. & Korshin, G. V. (1999). Separation of cesium from high ionic strength solutions using a cobalt hexacyanoferrate-modified graphite electrode. Environmental Science and Technology. 33(15), 2633-2637.

Project: 55171

Title: Development of Advanced In Situ Techniques for Chemistry Monitoring and Corrosion Mitigation in SCWO Environments

PI: Dr. Digby D. MacDonald *Institution:* Pennsylvania State University

Publication Type: Journal

Lvov, S. N., Zhou, X. Y., & Macdonald, D. D. (1999). Flow-through electrochemical cell for accurate pH measurements at temperatures up to 400°C. J. Electroanal. Chem. 463, 146-156.

Publication Type: Other

Lvov, S. N., Zhou, X. Y., Ulyanov, S. M., & Macdonald, S. N. (2000, in press). Potentiometric measurements of association constant and pH in high temperature HCI (aq) solutions. Tremaine, P. P. R., Hill, P. G., Irish, D. E., & Palakrishnan, P. V. (Eds.). Steam, Water, and Hydrothermal Systems: Physics and Chemistry. Meeting the Needs of Industry. Press Ottawa.

Zhou, X. Y., Lvov, S. N., & Ulyanov, S. M. (1998, Nov. 11). Safe Yttria-stabilized zirconia (YSZ) pH sensing electrode for high temperature aqueous systems. Invention Disclosure No. 98-1989.

Publication Type: Presentation

Lvov, S. N., et. al. (2000, Jun. 5). Reference systems for assessing viability and accuracy of pH sensors in high temperature subcritical and supercritical aqueous solutions. Chem. Geol. 167(1-2), 105-115.

Lvov, S. N., Zhou, X. Y., & Macdonald, S. N. (1998, May 3-8). Potentiometric pH measurements in supercritical aqueous solutions. The 193rd Meeting of the Electrochemical Society, Inc. Abstracts No. 1016. San Diego, CA.

Lvov, S. N., Zhou, X. Y., Wei, X. J., Ulyanov, S. M., & Macdonald, D. D. (1999, Aug. 22-26). Electrochemical corrosion studies in high temperature subcritical and supercritical aqueous environments. The 218th American Chemical Society Meeting, Abstract No. 129. New Orleans, LA.

Macdonald, D. D. (1997, May 11-14). Chemistry sensors for the universal solvents-supercritical aqueous solutions. Proceedings of the 4th International Symposium on Supercritical Fluids. Sendai, Japan. 861-864.

Macdonald, D. D. (1999, Nov. 10). The chemistry and electrochemistry of high subcritical and supercritical aqueous systems. Distinguished Lecturer Series, University of Toronto. Toronto, Canada.

Macdonald, D. D., Lvov, S. N., & Kriksunov, L. B. (1998, May 3-8). The chemical and electrochemical properties of supercritical aqueous solutions. The 193rd Meeting of the Electrochemical Society, Inc. Abstracts No. 1012. San Diego, CA.

Project: 59981

Title: Real-Time Broad Spectrum Characterization of Hazardous Waste by Membrane Introduction Mass Spectrometry

PI: Dr. Charles W. Wilkerson, Jr. *Institution:* Los Alamos National Laboratory

Publication Type: Presentation

Wilkerson Jr., C. W. (1999, Feb. 22-23). Workshop on harsh environment mass spectrometry. St. Petersburg, FL.

Wilkerson Jr., C. W. (1999, Feb. 28 - Mar. 4). WM99 - HLW, LLW, mixed wastes and environmental restoration - Working towards a cleaner environment. Tucson, AZ.

Wilkerson Jr., C. W. (1999, Mar. 7-12). Pittsburgh conference on analytical chemistry and applied spectroscopy. Orlando, FL.

Project: 60070

Title: The Development of Cavity Ringdown Spectroscopy as a Sensitive Continuous Emission Monitor for Metals

PI: Dr. George P. Miller *Institution:* Sensor Research and Developmenet Corporation

Publication Type: Journal

Miller, G. P. & Winstead, C. B. (1997). Inductively coupled plasma cavity ringdown spectroscopy. J. Anal. Atomic Spectro. 12, 907.

Winstead, C. B., Mazzotti, F. J., Mierzwa, J., & Miller, G. P. (1999, Jul.). Preliminary results for electrothermal atomization-cavity ringdown spectroscopy (ETA-CRDS). Anal. Commun. 36(7), 277-279.

Publication Type: Paper

Miller, G. P. (2000, in press). Determination of elemental mercury by cavity ringdown. Analyst.

Publication Type: Presentation

Miller, G. P. & Winstead, C. B. (1997, Jan. 12-17). ICP-cavity ringdown spectroscopy. Abstract O1-4, Winter Conference in Spectrochemistry. Gent, Belgium.

Miller, G. P. & Winstead, C. B. (1998, Oct. 12-15). ICP-cavity ringdown spectroscopy. Abstract 407, The 25th FACSS Conf. Austin, TX.

Miller, G. P. (2000, Sep. 25). Recent progress on analytical atomic cavity ringdown spectroscopy. FACSS conference, Nashville, TN.

Publication Type: Report

Miller, G. P. (2000, Oct.). Cavity ringdown laser absorption spectroscopy. In Meyers, R. A., Ed. Encyclopedia of Analytical Chemistry. Wiley & Sons, New York, NY.

Project: 73844 (Renewal of Project No. 60231)

Title: Miniature Chemical Sensor Combining Molecular Recognition with Evanescent-Wave Cavity Ring-Down Spectroscopy

PI: Dr. Andrew C. R. Pipino *Institution:* National Institute of Standards & Technology - Maryland

Publication Type: Journal

Pipino, A. C. R. (1998, Nov.). Evanescent wave cavity ring-down spectroscopy for ultra-sensitive chemical detection. SPIE 3535, 57. Boston, MA.

Pipino, A. C. R., et. al. (1997). Evanescent wave cavity ring-down spectroscopy with a total-internal-reflection minicavity. Rev. Sci. Instrum. 68, 2978.

Pipino, A.C.R., et. al. (1997). Evanescent wave cavity ring-down spectroscopy as a probe of surface processes. Chem. Phys. Lett. 280, 104.

Publication Type: Patent

Pipino, A. C. R. (1998, Nov. 10). Broad band intra-cavity total reflection chemical sensor. US #5,835,231.

Pipino, A. C. R. (1999, Aug. 24). Intra-cavity total reflection for high sensitivity measurement of optical properties. US #5,943,136.

Pipino, A. C. R. (1999, Nov. 16). Intra-cavity total reflection for high sensitivity measurement of optical properties. US #5,986,768.

Engineering Science

Project: 54973

Title: A Novel Energy-Efficient Plasma Chemical Process for the Destruction of Volatile Toxic Compounds

PI: Dr. Lal A. Pinnaduwage *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Ding, W., McCorkle, D. L., & Pinnaduwage, L. A. (1998). Enhanced negative ion formation by electron attachment to highly-excited molecules in a flowing plasma. J. Appl. Phys. 84, 3051.

Ding, W., Pinnaduwage, L. A., Tav, C., & McCorkle, D. L. (1999). The role of high Rydberg states in enhanced o-formation in a pulsed O2 discharge. Plasma Sources Sci. Technol. 8, 384.

Ma, C. Y., McCorkle, D. L., Ding, W., & Pinnaduwage, L. A. (1999). A methodology for direct sampling and gas chromatographic/mass spectral analysis of volatile organic compounds emerging from a low pressure, flow-through reaction cell. J. Chromatography A. 844, 217.

Mabel, A. M., Lin, S. H., & Pinnaduwage, L. A. (1998). Potential energy surfaces of H2. Chem. Phys. Lett. 285, 114.

McCorkle, D. L., Ding, W. X., Ma, C. Y. & Pinnaduwage, L. A. (1999). Dissociation of benzene in a
pulsed glow discharge. J. Appl. Phys. 86, 3550.

McCorkle, D. L., Ding, W., Ma, C. Y., & Pinnaduwage, L. A. (1999). Exploratory studies on a plasma remediation process based on enhanced dissociative electron attachment to highly-excited molecules. J. Phys. D. 32, 46.

Pinnaduwage, L. A. & Datskos, P. G. (1997, Jun. 15). Electron attachment to excited states of silane: Implications for plasma processing discharges. J. Appl. Phys. 81(12), 7715-7727.

Pinnaduwage, L. A., et. al. (1999). Enhanced electron attachment to Rydberg states in molecular hydrogen volume discharges. J.Appl. Phys. 85, 7064.

Pinnaduwage, L. A., McCorkle, D. L., & Ding, W. (1997). Enhanced electron attachment to highly excited molecules using a plasma mixing scheme. Appl. Phys. Lett. 71, 3634.

Pinnaduwage, L. A., Tav, C., McCorkle, D. L., & Ding, W. (1999). Temperature dependence of electron attachment to methylene chloride. J. Chem. Phys. 110, 9011.

Publication Type: Patent

Pinnaduwage, L. A. (1999, Apr. 20). Plasma mixing glow discharge device for analytical applications. US Patent #5,896,196.

Publication Type: Presentation

Ding, W. X., McCorkle, D. L., & Pinnaduwage, L. A. (1998, Jun. 1-4). Decomposition of volatile organic compounds in a positive column glow discharge plasma. Presentation at the 25th IEEE International Conference on Plasma Science. Raleigh, NC.

Ding, W. X., Pinnaduwage, L. A., Tav, C., & McCorkle, D. L. (1999, Mar. 20-26). O- formation by electron attachment to high Rydberg states. Presented at the 1999 Centennial Meeting of the American Physical Society. Atlanta, GA.

Ding, W., Ma, C. Y., McCorkle, D. L., & Pinnaduwage, L. A. (1998, Jun. 1-4). Decomposition of volatile organic compounds in a positive column glow discharge plasma. Presented at the 25th IEEE International Conference on Plasma Science. Raleigh, NC.

Ding, W., McCorkle, D. L., & Pinnaduwage, L. A. (1998, Jun. 1-4). Enhanced radical formation by electron attachment to highly-excited states of molecules in plasmas. Presented at the 25th IEEE International Conference on Plasma Science. Raleigh, NC.

Ding, W., McCorkle, D. L., Ma, C. Y., & Pinnaduwage, L. A. (1999, Oct. 5-8). Dissociation of benzene in a pulsed glow discharge. 52nd Annual Gaseous Electronics Conference. Norfolk, VA.

Ma, C. Y., McCorkle, D. L., Ding, W., & Pinnaduwage, L. A. (1998, May 31 - Jun. 4). Methodology for direct sampling of volatile organic compounds emerging from a low-pressure, flow-through reaction cell for subsequent GC-GC/MS analysis. Presented at the 46th ASMS Conference on Mass Spectrometry and Allied Topics. Orlando, FL.

McCorkle, D. L. & Pinnaduwage, L. A. (1997, Oct. 6-9). Destruction of CH2Cl2 using a glow discharge scheme. 50th Annual Gaseous Electronics Conference. Madison, WI.

Pinnaduwage, L. A. (1997, Jun. 29 - Jul. 2). Implications of electron attachment to highly-excited states in pulsed power discharges. 11th IEEE Pulsed Power Conference. Baltimore, MA.

Pinnaduwage, L. A. (1999, Sep. 22). Novel energy-efficient plasma chemical process for the destruction of volatile toxic compounds. DOE Environmental Management Science Program Workshop. Oak Ridge, TN.

Pinnaduwage, L. A., Datskos, P. G., Ding, W. X., & McCorkle, D. L. (1998, Jun. 27 - Jul. 3). Enhanced electron attachment to highly-excited states of molecules: Implications for plasma processing discharges. Presentation at the 1998 International Congress on Plasma Physics. Prague, Czech Republic.

Pinnaduwage, L. A., Ding, W. X., & McCorkle, D. L. (1999, Mar. 20-26). Enhanced electron attachment to Rydberg states in molecular hydrogen volume discharges. Presented at the 1999 Centennial Meeting of the American Physical Society. Atlanta, GA.

Pinnaduwage, L. A., Ding, W. X., & McCorkle, D. L. (1998, Jun. 27 - Jul. 3). Enhanced electron attachment to superexcited Rydberg states of molecular hydrogen using a plasma mixing scheme. Presented at the 1998 International Congress on Plasma Physics. Prague, Czech Republic.

Pinnaduwage, L. A., Ding, W. X., McCorkle, D. L., & Ma, C. Y. (1999, Jun. 27-30). Implications of electron attachment to highly-excited states of molecules and its applications in pulsed plasmas. 12th IEEE Pulsed Power Conference. Monterrey, CA.

Pinnaduwage, L. A., Ding, W., & McCorkle, D. L. (1999, Oct. 5-8). Negative ion formation in pulsed plasmas. 52nd Annual Gaseous Electronics Conference. Norfolk, VA.

Pinnaduwage, L. A., Ma, C. Y., McCorkle, D. L., & Ding, W. (1998, Jul. 27-30). A novel energy-efficient plasma chemical process for the destruction of volatile toxic compounds. Presented at the Environmental Management Science Program Workshop. Chicago, IL.

Tav, C. & Pinnaduwage, L. A. (1999, Oct. 5-8). Dissociative electron attachment to laser-excited benzene. 52nd Annual Gaseous Electronics Conference. Norfolk, VA.

Publication Type: Proceeding

Pinnaduwage, L. A. (1997). Implications of electron attachment to highly-excited states in pulsed power discharges. Cooperstein, G. & Vitkovitsky, I. (Eds.). Digest of Technical Papers of the 11th IEEE Pulsed Power Conference. IEEE Publishing Services. New York, NY. 1048-1053.

Pinnaduwage, L. A., Datskos, P. G., Ding, W. X., & McCorkle, D. L. (1999). Enhanced electron attachment to highly-excited states of molecules: Implications for plasma processing discharges. Pavlo, P. (Ed.). Proceedings of the 1998 International Congress on Plasma Physics. 125-128.

Pinnaduwage, L. A., Ding, W. X., & McCorkle, D. L. (1999). Enhanced electron attachment to superexcited Rydberg states of molecular hydrogen using a plasma mixing scheme. Pavlo, P. (Ed.). Proceedings of the 1998 International Congress on Plasma Physics. 129-132.

Pinnaduwage, L. A., Ding, W. X., McCorkle, D. L., & Ma, C. Y. (1999). Enhanced electron attachment to highly-excited molecules and its applications in pulsed plasmas. Stallings, C. & Kirbie, H. (Eds.). Digest of Technical Papers of the 12th IEEE Pulsed Power Conference. IEEE Publishing Services. New York, NY. 1322-1325

Publication Type: Theses/Dissertations

Tav, C. (2000). Enhanced electron attachment to vibrationally and electrically excited molecules. Ph. D. dissertation.

Project: 60155

Title: Measurements and Models for Hazardous Chemical and Mixed Wastes
PI: Dr. Cynthia Holcomb *Institution:* National Institute of Standards & Technology - Boulder

Publication Type: Journal

Mathias, P. M., Naheiri, T., & Oh, E. M. (1989). A density correction for the Peng-Robinson equation of state. Fluid Phase Equilibria. 47, 77-87.

Inorganic Chemistry

Project: 54506

Title: Acid-Base Behavior in Hydrothermal Processing of Wastes
PI: Dr. Keith P. Johnston *Institution:* University of Texas at Austin

Publication Type: Journal

Chlistunoff, J. B., Ziegler, K. J., Lasdon, L., & Johnston, K. P. (1999). Nitric/nitrous acid equilibria in supercritical water. Journal of Phys. Chem. B. 103, 1678-1688.

Johnston, K. P. & Chlistunoff, J. B. (1998). Neutralization of acids and bases in subcritical and supercritical water: Acetic acid and HCl. J. Supercrit. Fluid. 12, 155-64.

Ziegler, K. J., Lasdon, L., Chlistunoff, J., & Johnston, K. P. (1999). Optimization models for determining nitric acid equilibria in supercritical water. Comput. Chem. 23(5), 421-434.

Publication Type: Report

Johnston, K. P. & Rossky, P. J. (1999, in press). Solution chemistry in supercritical water: spectroscopy and simulation. E. Kiran (Ed.), NATO Adv. Study Institute on Supercritical Fluids.

Project: 55276

Title: Fundamental Chemistry and Thermodynamics of Hydrothermal Oxidation Processes

PI: Dr. John M. Simonson *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Blencoe, J. G., Anovitz, L. M., & Seitz, J. C. (1998, in press). A new method for modeling the thermodynamic mixing properties of high-temperature H2 O-CO2 fluids. Eos. 79.

Blencoe, J. G., Seitz, J. C., & Anovitz, L. M., (1999, in press). The CO2 -H2 O System. II. Calculated Thermodynamic Mixing Properties for 400°C, 0-400 MPa. Geochim. Cosmochim. Acta. 63.

Chialvo, A. A., Cummings, P. T., Simonson, J. M., & Mesmer, R. E. (1999, Jan. 8). Solvation in high-temperature electrolyte solutions. II. Some formal results. J. Chem. Phys. 110(2), 1075-1086.

Chialvo, A. A., Cummings, P. T., Simonson, J. M., & Mesmer, R. E. (1999, Jan. 8). Solvation in high-temperature electrolyte solutions. I. Hydration shell behavior from molecular simulation. J. Chem. Phys. 110(2), 1064-1074.

Chialvo, A. A., Cummings, P. T., Simonson, J. M., & Mesmer, R. E. (1998). Thermodynamics and kinetics of ion speciation in supercritical aqueous solutions: A molecular-based study. Fluid Phase Equilibria. 150-151, 107-115.

Chialvo, A. A., Kusalik, P.G., Cummings, P. T., Simonson, J. M., & Mesmer, R. E. (2000, Apr. 17.). Molecular approach to high temperature solvation. Formal, integral equation, and experimental results. J. Phys-Condens. Mat. 12(15), 3585-3593.

Dai, S., Burleigh, M., Simonson, J. M., Mesmer, R. E., & Xue, Z. -L. (1998). Application of chemometric methods in UV-Vis absorption spectroscopic studies of uranyl ion dimerization reaction in aqueous solutions. Radiochimica Acta. 81, 195-199.

Moore, R. C., Mesmer, R. E., & Simonson, J. M. (1997). The solubility of potassium carbonate in water between 384 and 529 K measured using the synthetic method. J. Chem. Eng. Data. 42, 1078-1081.

Seitz, J. C. & Blencoe, J. G. (1999, in press). The CO2 -H2 O System. I. Experimental Determination of Volumetric Properties at 400°C, 10-100 MPa. Geochim. Cosmochim. Acta. 63.

Publication Type: Presentation

Blencoe, J. G., Anovitz, L. M. & Seitz, J. C. (1998). A Helmholz free energy model for supercritical H2 O-CO2 mixtures. Geol. Soc. Amer. Abs. with Prog. 30, A-319.

Blencoe, J. G., Anovitz, L. M., Seitz, J. C. (1997). Serious shortcomings of semi-empirical equations of state for high-temperature aqueous C-O-H-N fluids. Geol. Soc. Amer. Abs. with Prog. 29, A-210.

Seitz, J. C. & Blencoe, J. G. (1997). Experimentally determined volumetric properties and solvus relations for H2 O-CO2 -N2 mixtures at 300°C and pressures < 1000 bars. Geol. Soc. Amer. Abs. with Prog. 29, A-209.

Singh, J., Blencoe, J. G., & Seitz, J. C., (1998). Experimentally determined excess molar volumes for H2 O-N2 fluids at 300°C, 75-1000 bars. Geol. Soc. Amer. Abs. with Prog. 30, A-319.

Project: 59934

Title: Hazardous Gas Production by Alpha Particles in Solid Organic Transuranic Waste Matrices

PI: Dr. Jay A. LaVerne *Institution:* University of Notre Dame

Publication Type: Journal

Chang, Z. & La Verne, J. A. (2000). Hydrogen production in the heavy ion radiolysis of polymers: I. Polyethylene, polypropylene, poly(methyl methacrylate) and polystyrene. J. Phys. Chem. B. 104, 10557-10562.

Chang, Z. & LaVerne, J. A. (1999). Molecular hydrogen production in the radiolysis of high density polyethylene. J. Phys. Chem. B. 103, 8267-8271.

Chang, Z. & LaVerne, J. A. (1999). The yield of hydrogen gas in the gamma-ray and heavy-ion radiolysis of high density polyethylene. J. Phys. Chem. B. 103, 8267-8271.

Chang, Z. & LaVerne, J. A. (2000). Hydrogen production in the heavy ion radiolysis of polyethylene, polypropylene, poly(methyl methacrylate) and polystyrene. J. Poly. Sci. A. Poly. Chem. 38, 1656-1661.

Chang, Z. & LaVerne, J. A. (2000). Hydrogen production in y-ray and helium ion radiolysis of polyethylene, polypropylene, poly(methyl-methacrylate) and polystyrene. J. Poly. Sci. 38, 000-000.

Chang, Z. & LaVerne, J. A. (2001, in press). The gases produced in the gamma and heavy-ion radiolysis of poly(methyl methacrylate). Radiat. Phys. Chem.

LaVerne, J. A., Chang, Z., & Araos, M. S. (2001, in press). Heavy ion radiolysis of organic materials. Radiat. Phys. Chem.

Publication Type: Poster

Chang, Z. (1999, Aug. 21-25). Production of hydrogen gas in the heavy-ion radiolysis of high-density polyethylene. 218th American Chemical Society National Meeting. New Orleans, LA.

LaVerne, J. A. & Chang, Z. (1999, Aug. 21-25). Hydrogen production in the radiolysis of polymers. 218th American Chemical Society National Meeting. New Orleans, LA.

LaVerne, J. A. & Chang, Z. (2000, Jun. 25-30). Production of hydrogen in the heavy ion radiolysis of polymers. Gordon Conference on Radiation Chemistry. Plymouth, NH.

Publication Type: Presentation

LaVerne, J. A. (2000, Mar. 14). Heavy ion radiolysis of organic materials. Invited presentation at the International Symposium on Prospects for Application of Radiation Towards the 21st Century. Waseda University. Waseda, Japan.

Materials Science

Project: 55387

Title: Photooxidation of Organic Waste Using Semiconductor Nanoclusters

PI: Dr. Jess P. Wilcoxon *Institution:* Sandia National Laboratories - Albuquerque

Publication Type: Journal

Parsapour, F., Kelley, D. F., Craft, S., & Wilcoxon, J. P. (1996). Electron transfer dynamics in MoS2 nanoclusters: Normal and inverted behavior. J. Chem. Phys. 104, 1.

Thurston, T. R. & Wilcoxon, J. P. (1998). Photo-oxidation of organic chemicals catalyzed by nanoscale MoS2. J. Phys. Chem. 103, 11.

Wilcoxon, J. P., Newcomer, P., & Samara, G. A. (1997). Synthesis and optical properties of MoS2 and isomorphous nanoclusters in the quantum confinement regime. J. Appl. Phys. 81, 7934.

Publication Type: Patent

Wilcoxon, J. P. (1999, Jan.). Visible light photooxidation of toxic organic chemicals using nanoscale MoS2. DOE Technical Advance Patent Application filed Jan. 1999.

Publication Type: Proceeding

Wilcoxon, J. P. & Thurston, T. R. (1998). Photocatalysis using nanosize semiconductors. Proceedings of Symposium FF, Fall MRS Meeting. Boston, MA.

Wilcoxon, J. P., Parsapour, R., & Kelley, D. F. (1997, May 4-9). Studies of photoredox reactions on nanosize semiconductors. 4th International Conference on Quantum Confinement: Nanoscale Materials, Devices, and Systems. 119th Meeting of the Electrochemical Society. Montreal, Quebec, Canada.

Microbial Science

Project: 73833 (Renewal of Project No. 60150)

Title: Genetic Engineering of a Radiation-resistant Bacterium for Biodegradation of Mixed Wastes

PI: Dr. Mary E. Lidstrom *Institution:* University of Washington

Publication Type: Poster

Meima, R., Rothfuss, H., Gewin, L., & Lidstrom, M. E. (1998, Jul. 27-30). Genetic engineering of a radiation-resistant bacterium for biodegradation of mixed wastes. Poster presentation at the DOE Environmental Management Science Program Workshop. Chicago, IL.

Separations Chemistry

Project: 54571

Title: Removal of Heavy Metals and Organic Contaminants from Aqueous Streams by Novel Filtration Methods

PI: Dr. Nelly M. Rodriguez

Institution: Northeastern University

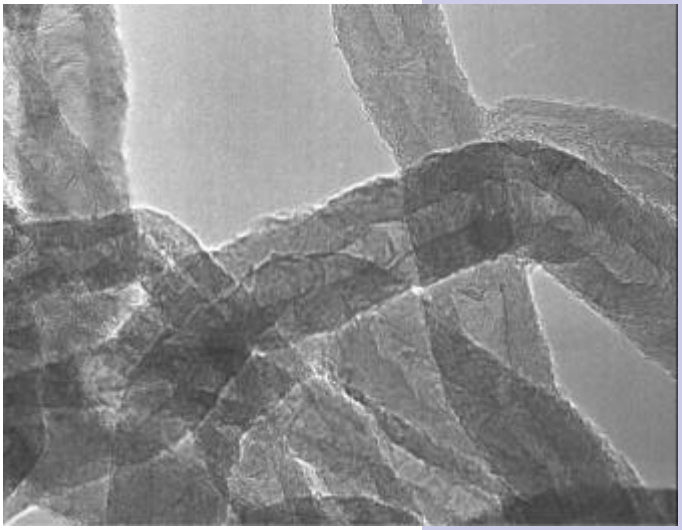
Publication Type: Journal

Anderson, P. E. & Rodriguez, N. M. (1999). Synthesis of graphite nanofibers from the decomposition of CO/H2 over silica supported iron-nickel particles. J. Mat. Res. 14, 2912.

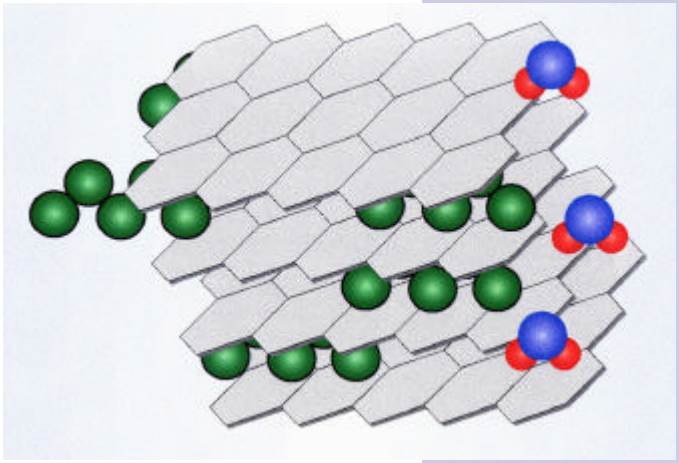
Anderson, P. E. & Rodriguez, N. M. (1999, Jul.). Growth of graphite nanofibers from the decomposition of CO/H2 over silica supported iron-nickel particles. J. Mater. Res. 14(7), 2912-2921.

Anderson, P. E. & Rodriguez, N. M. (2000). Synthesis of graphite nanofibers over transition metal catalysts supported on various substrates. Chem. Of Mat. 12, 823.

Anderson, P. E. & Rodriguez, N. M. (2000, in press). Effect of the support on the synthesis of carbon nanofibers. Mat. Res. Soc. Symp. Proc.



Transmission electron micrograph (TEM) of carbon nanofibers. [see Project #54571]



Organic impurity molecules being trapped between the graphene layers of a carbon nanofiber. Water molecules are preferentially absorbed at the edge sites of the structure. [see Project #54571]

Anderson, P. E., Engel, E., Crowe, A., Park, C., & Rodriguez, N. M. (2000, Mar.). Influence of the support on the structural characteristics of carbon nanofibers produced from the metal-catalyzed decomposition of ethylene. Chem. Mater. 12(3), 823-830.

Park, C., Anderson, P. E., & Chambers, A. (1999, Dec. 2). Further studies of the interaction of hydrogen with graphite nanofibers. J. Phys. Chem. B. 103(48), 10572-10581.

Park, C., Engel, E., Crowe, A., Gilbert, T. R., & Rodriguez, N. M. (2000, in press). Removal of organic molecules from aqueous solutions using graphite nanofibers. Langmuir.

Publication Type: Proceeding

Anderson, P. E., Engel, E., Crowe, A., Park, C., & Rodriguez, N. M. (2000). Carbon nanofibers for environmental applications. Proceedings of the WM2000 Conference. Tucson, AZ.

Project: 54770

Title: New Anion-Exchange Resins for Improved Separations of Nuclear Materials
PI: Dr. Mary E. Barr *Institution:* Los Alamos National Laboratory

Publication Type: Journal

Marsh, S. F., Jarvinen, G. D., & Bartsch, R. A. (1997). New bifunctional anion-exchange resins for nuclear waste treatment. Reactive Polymers. 35, 75-80.

Marsh, S. F., Jarvinen, G. D., Bartsch, R. A., Nam, J., & Barr, M. E. (1998). New bifunctional anion-exchange resins for nuclear waste treatment-II. J. Radioanal. Nucl. Chem. 235, 37-40.

Publication Type: Presentation

Barr, M. E., Jarvinen, G. D., Marsh, S. F., & Bartsch, R. A. (1997, Apr. 13). Development of anion-exchange resins for separations of actinides. Abstracts of Papers of the American Chemical Society. 213(pt.2), 73-IEC.

Barr, M. E., Jarvinen, G. D., Moody, E. W., & Vaughn, R. B. (1998, Aug. 23). Sorption of Pu(IV) by soluble anion-exchange polymers. Abstracts of Papers of the American Chemical Society. 216(pt.2), 88-NUCL, & 216(pt.1), 5-TECH.

Barr, M. E., Jarvinen, G. D., Schulte, L. D., Stark, P. C., & Chamberlin, R. M. (1999, Mar. 21). Americium separations from complex mixtures using anion exchange. Abstracts of Papers of the American Chemical Society. 217, 019-IEC.

Bartsch, R. A., et. al. (1999, Mar. 21). Sorption of Pu(IV) from nitric acid by bifunctional anion-exchange resins. Abstracts of Papers of the American Chemical Society. 217, 125-IEC.

Marsh, S. F., Jarvinen, G. D., Bartsch, R. A., Nam, J., & Barr, M. E. (1997, Apr.). New bifunctional anion-exchange resins for nuclear waste treatment. Marc IV conference on Radioanalytical Chemistry, Kona, HI.

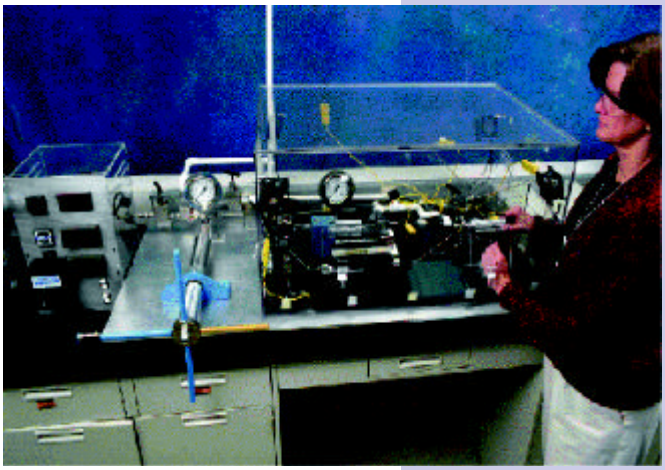
Moody, E. W., Barr, M. E., & Jarvinen, G. D. (1999). QSAR of distribution coefficients for actinide hexanitrato complexes. Abstracts of Papers of the American Chemical Society. 217(pt.2), 170-NUCL.

Project: 54847

Title: Photocatalytic and Chemical Oxidation of Organic Compounds in Supercritical Carbon Dioxide
PI: Dr. Daniel M. Blake
Institution: National Renewable Energy Laboratory

Publication Type: Journal

Jacoby, W. A., et al. (1996). Heterogeneous photocatalysis for control of volatile organic compounds in indoor air. J. Air Waste Manage. Assoc. 46(9), 891-898.



A National Renewable Energy Laboratory project uses an experimental system to study photocatalytic oxidation of organic substances in supercritical carbon dioxide. Organic compounds are monitored by an online gas chromatograph or by UV-visible spectroscopy. [see Project #54847]

Project: 54942

Title: Spectroscopy, Modeling and Computation of Metal Chelate Solubility in Supercritical CO_2
PI: Dr. Joan F. Brennecke
Institution: University of Notre Dame

Publication Type: Journal

Brennecke, J. F. & Chateauneuf, J. E. (1999). Homogeneous organic reactions as mechanistic probes in supercritical fluids. Chemical Reviews. 99(2), 433-452.

Hua, J. Z., Brennecke, J. F., & Stadtherr, M. A. (1998). Enhanced interval analysis for phase stability: Cubic equation of state models. Ind. Eng. Chem. Res. 37, 1519-1527.

Hua, J. Z., Brennecke, J. F., & Stadtherr, M. A. (1998). Reliable computation of phase stability using interval analysis: Cubic equation of state models. Computers and Chemical Engineering. 22, 1207-1214.

Hua, J. Z., Maier, R. W., Tessier, S. R., Brennecke, J. F., & Stadtherr, M. A. (1999). Interval analysis for thermodynamic calculations in process design: A novel and completely reliable approach. Fluid Phase Equilibria, 158-160, 607-615.

Maier, R. W., Brennecke, J. F., & Stadtherr, M. A. (1998). Reliable computation of homogeneous azeotropes. AIChE J. 44, 1745-1755.

Maier, R. W., Brennecke, J. F., & Stadtherr, M. A. (1999, in press). Computing homogeneous azeotropes using interval analysis. Chem. Eng. & Tech.

Stadtherr, M. A. (1999). High performance computing: Are we just getting wrong answers faster? AIChE CAST Communications. 22(1), 6-14.

Tessier, S. R., Brennecke, J. F., & Stadtherr, M. A. (1999, in press). Reliable phase stability analysis for excess Gibbs energy models. Chemical Engineering Science.

Xu, G., Scurto, A. M., Castier, M., Brennecke, J. F., & Stadtherr, M. A. (1999, in press). Reliable computation of high pressure solid-fluid equilibrium. Ind. Eng. Chem. Res.

Publication Type: Poster

Chateauneuf, J. E. (1999, Aug. 23). The use of reaction intermediates to probe supercritical fluid solvent effects. American Chemical Society 218th National Meeting. New Orleans, LA.

Chateauneuf, J. E., Zhang, J., Brink, J., Slominis, M., & Perkovic, M. (1999, Mar. 24). Investigation of free radical ion reactivity with supercritical carbon dioxide. Physical Chemistry Division, Free Radicals in the Condensed Phase Symposium. American Chemical Society 217th National Meeting. Anaheim, CA.

Chateauneuf, J. E., Zhang, J., Brink, J., Slominis, M., & Perkovic, M. (1999, Mar. 22). Investigation of free radical and radical ion reactivity with supercritical carbon dioxide. Poster presentation at the Sci-Mix Division of the American Chemical Society 217th National Meeting, Anaheim, CA.

Hua, J. Z., Maier, R. W., Tessier, S. R., Brennecke, J. F., & Stadtherr, M. A. (1998, Apr. 26 - May 1). Interval analysis for thermodynamic calculations in process design: A novel and completely reliable approach. Eighth International Conference on Properties and Phase Equilibria for Product and Process Design. Noordwijkerhout, The Netherlands.

Publication Type: Presentation

Brennecke, J. F. & Stadtherr, M. A. (1999, May 27). Reliable computation of phase behavior using interval analysis. Escola de Quimica, Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil.

Brennecke, J. F. (1997, Nov. 6). Supercritical fluids for environmental applications: A chemical engineering perspective. Department of Chemistry, Western Michigan University, Kalamazoo, MI.

Brennecke, J. F. (1998, Apr. 13-16). Dense phase fluids: Phase behavior. Department of Energy/Environmental Protection Agency Dense Phase Fluids and Alternative Reaction Media Workshop, Santa Fe, NM.

Brennecke, J. F. (1998, Apr. 16). Thermodynamic and kinetic studies in supercritical fluids. Department of Chemistry, Loyola University of Chicago, Chicago, IL.

Brennecke, J. F. (1998, Oct. 1). Using spectroscopy to understand metal chelates in supercritical CO2. Department of Chemical Engineering, University of Massachussettes, Amherst, MA.

Brennecke, J. F. (1998, Sep. 9). Understanding metal chelates in supercritical CO2. Department of Chemical Engineering, University of Texas at Austin, Austin, TX.

Brennecke, J. F. (1999, Apr. 10-13). Spectroscopy to measure solvation, kinetics, and equilibrium in supercritical fluids. 6th Meeting on Supercritical Fluids: Chemistry and Materials, Nottingham, U. K.

Brennecke, J. F. (1999, Apr. 30). Polution prevention with supercritical CO2. Department of Civil Engineering, Northwestern University, Evanston, IL.

Brennecke, J. F. (1999, Jun. 1). Spectroscopic measurements of local compositions. PLAPIQUI, Universidad Nacional del Sur, Bahia Blanca, Argentina.

Brennecke, J. F. (1999, Jun. 4). Application of supercritical chemical engineering processes in environmental protection and remediation. PLAPIQUI, Universidad Nacional del Sur, Bahia Blanca, Argentina.

Brennecke, J. F. (1999, May 25). Environmental applications of supercritical fluids. Escola de Quimica, Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil.

Brennecke, J. F., Stadtherr, M. A., & Chateauneuf, J. E. (1998, Jul. 27-30). Spectroscopy, modeling, and computation of metal chelate solubility in supercritical CO2. Department of Energy EMSP Scientific Workshop, Rosemont, IL.

Chateauneuf, J. E. (1998, Mar. 1). The use of reaction intermediates to investigate supercritical fluid solvent effects: The development of supercritical fluids as environmentally benign reaction media. Department of Chemistry, Central Michigan University, Mt. Pleasant, MI.

Chateauneuf, J. E. (1999, Aug. 22-26). The use of reaction intermediates to probe supercritical fluid solvent effects. Symposium on Chemistry of Reactive Intermediates and Modeling in Hydrocarbon Conversion. American Chemical Society 218th National Meeting. New Orleans, LA.

Chateauneuf, J. E. (1999, Jul. 11-16). Free radical reactions in supercritical fluids. Gordon Research Conference on Free Radical Reactions, Holderness School, Plymouth, NH.

Chateauneuf, J. E. (1999, Jun. 30). Reactions in supercritical fluids: The development of supercritical fluids as environmentally benign reaction media. Department of Chemistry, Argonne National Laboratory, Argonne, IL.

Chateauneuf, J. E. (1999, Mar. 3). The development of supercritical fluids as environmentally benign reaction media: The influence of SCF solvation on chemical reactivity. Department of Chemistry and the Center for Photochemical Sciences, Bowling Green State University, Bowling Green, OH.

Chateauneuf, J. E. (1999, May 19). Reactions in supercritical fluids: The development of supercritical fluids as environmentally benign reaction media. Department of Chemistry, Andrews University, Berrien Springs, MI.

Hua, J. Z., Brennecke, J. F., & Stadtherr, M. A. (1997, Nov. 16-21). Combined local and global approach to reliable computation of phase eqilibria. Annual AIChE Meeting. Los Angeles, CA.

Maier, R. W., Brennecke, J. F., & Stadtherr, M. A. (1998, Nov. 15-20). Computation of reactive azeotropes using interval analysis. Annual AIChE Meeting. Miami, FL.

Maier, R. W., Brennecke, J. F., & Stadtherr, M. A. (1999, Oct. 31-Nov. 5). A new approach for reliably computing all azeotropes of multicomponent mixtures. Annual AIChE Meeting. Dallas, TX.

Maier, R. W., Brennecke, J. F., & Stadtherr, M. A. (1997, Nov. 16-21). A new approach for reliable computation of homogenous azeotropes in multicomponent mixtures. AIChE Annual Meeting. Los Angeles, CA.

Maier, R. W., Stadtherr, M. A., & Brennecke, J. F. (1998, May 18-19). Reliable computation of homogenous azeotropes. 1998 Midwest Thermodynamics and Statistical Mechanics Conference. Notre Dame, IN.

Roggeman, E. J., Scurto, A. M., Brennecke, J. F., & Chateauneuf, J. E. (1998, May 18-19). Spectroscopic measurements of preferential solvation and novel solubility measurements of metal chelate complexes in pure and modified supercritical CO2. 1998 Midwest Thermodynamics and Statistical Mechanics Conference. Notre Dame, IN.

Roggeman, E. J., Scurto, A. M., Chateauneuf, J. E., & Brennecke, J. F. (1998, Nov. 15-20). Cosolvent effects to enhance metal extraction with supercritical CO2. Annual AIChE Meeting. Miami, FL.

Roggeman, E. J., Scurto, A. M., Stadherr, M. A., & Brennecke, J. F. (1998, Jul. 12-16). Spectroscopy, measurement, and modeling of metal chelate solubility in supercritical CO2. 8th International Symposium on Supercritical Fluid Chromatography and Extraction, St. Louis, MO.

Stadtherr, M. A. (1998, Feb. 24). Reliable process modeling using interval analysis. Department of Chemical Engineering Seminar, Carnegie-Mellon University, Pittsburgh, PA.

Stadtherr, M. A. (1998, Nov. 15-20). High performance computing: Are we just getting wrong answers faster? Computing and Systems Technology Division Awards Dinner, AIChE Annual Meeting, Miami Beach, FL.

Stadtherr, M. A. (2000, Feb. 6-11). Recent advances in reliable nonlinear equation solving. Aspen World 2000. Orlando, FL.

Stadtherr, M. A. (2000, Mar. 29). Reliable process modeling using interval analysis. Department of Chemical Engineering Seminar. University of Kansas, Lawrence, KS.

Stadtherr, M. A., Hua, J. Z., & Brennecke, J. F. (1997, Oct. 26-29). Phase stability analysis for equation of state models. Institute for Operations Research and the Management Sciences, National Meeting, Dallas, TX.

Stadtherr, M. A., Maier, R. W., & Gau, C.-Y. (1999, Oct. 31-Nov. 5). New interval methodologies for reliable process modeling. AIChE Annual Meeting. Dallas, TX.

Stadtherr, M. A., Maier, R. W., Stradi, B. A., Xu, G., & Brennecke, J. F. (1998, Nov. 15-20). Reliable computation of high pressure phase behavior. Annual AIChE Meeting. Miami, FL.

Stadtherr, M. A., Xu, G., Stradi, B., Maier, R. W., & Brennecke, J. F. (1999, May 12-15). Reliable computation of phase behavior using interval methods. SIAM Annual Meeting, Atlanta, GA.

Xu, G., Brennecke, J. F., & Stadtherr, M. A. (1999, Oct. 31-Nov. 5). Reliable computation of solid-supercritical fluid equilibria using interval analysis. Annual AIChE Meeting. Dallas, TX.

Xu, G., Brennecke, J. F., & Stadtherr, M. A. (1999, May 17-18). Reliable computation of solid-fluid equilibria using interval analysis. Midwest Thermodynamics and Statistical Mechanics Conference. Detroit, MI.

Xu, G., Scurto, A. M., Castier, M., Stadtherr, M. A., & Brennecke, J. F. (2000, Apr. 8-12). Reliable computation of high pressure solid-fluid equilibrium. 5th International Symposium on Supercritical Fluids. Atlanta, GA.

Xu, G., Scurto, A. M., Castier, M., Stadtherr, M. A., & Brennecke, J. F. (2000, Sep. 24-27). Reliable computation of high pressure solid-fluid equilibrium. Presented in conjunction with Western Michigan University (subcontract) at COBEQ 2000. Aguas de Sao Pedro, Brazil.

Zhang, J., Roggeman, E. J., Chateauneuf, J. E., & Brennecke, J. F. (1997, Nov. 16-21). Cosolvent effects on metal chelates in supercritical CO2. Annual AIChE Meeting. Los Angeles, CA.

Publication Type: Proceeding

Kremer, M. J., et. al. (1999, Apr. 10-13). Spectroscopy to measure solvation, kinetics, and equilibrium in supercritical fluids. Proceedings of the 6th Meeting on Supercritical Fluids: Chemistry and Materials. Nottingham, U. K.

Roggeman, E. J., Scurto, A. M., Stadtherr, M. A., & Brennecke, J. F. (1998, Jul. 12-16). Spectroscopy, measurement and modeling of metal chelate solubility in supercritical CO2. Proceedings of the 8th International Symposium on Supercritical Fluid Chromatography and Extraction, St. Louis, MO.

Publication Type: Theses/Dissertations

Jin, H. (1999, Jul.). Spectroscopic investigations of carbocation reactivity in supercritical carbon dioxide. M. S. Thesis.

Zhang, J. (expected 2000). M. S. Thesis.

Project: 55103

Title: Utilization of Kinetic Isotope Effects for the Concentration of Tritium
PI: Dr. Gilbert M. Brown *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Huynh, M. H. V., El-Samonody, E-S., Meyer, T. J., & White, P. S. (1999, Aug. 23). The effect of stepwise oxidation on molecular structure in osmium hydrazido complexes. Inorg. Chem. 38(17), 3760+.

Huynh, M. H. V., et. al. (1999). Oxo-like reactivity of high oxidation state osmium hydrazido complexes. Journal of American Chemical Society. 121, 1403-1404.

Huynh, M. H. V., White, P. S., & Meyer, T. J. (1999, May 12). Proton-coupled electron transfer from nitrogen: A N-H/N-D kinetic isotope effect of 41.4. J. Am. Chem. Soc. 121(18), 4530-4531.

Lebeau, E. L. & Meyer, T.J. (1999). Oxidation of benzyl alcohol by a dioxo complex of Ru(VI). Inorganic Chemistry. 38, 2174-2181.

Trammell, S. A., et. al. (1998). Mechanisms of surface electron transfer: Proton-coupled electron transfer. Journal of American Chemical Society. 120, 13248-13249.

Publication Type: Proceeding

Barton, J. W., Klasson, K. T., & Davison, B. H. (1997). Extended operation and control of biomass overgrowth in biofiliters designed for VOC removal. Proceedings of the 90th Annual Meeting & Exhibition of Air and Waste Management Association. Toronto, Ontario, Canada.

Project: 60096

Title: Rational Synthesis of Imprinted Organofunctional Sol-Gel Materials for Toxic Metal Separation

PI: Dr. Ziling Benjamin Xue *Institution:* University of Tennessee at Knoxville

Publication Type: Journal

Dai, S., et. al. (1999). Imprint coating: Novel synthesis of selective functionalized ordered mesoporous sorbents. Angew. Chem. Int. Ed. 38, 1235-1239.

Dai, S., et. al. (1999, Oct. 1). A new methodology to functionalize surfaces of ordered mesoporous materials based on ion exchange reactions. Adv. Mater. 11(14), 1226-1230.

Shin, Y. S., Burleigh, M. C., Dai, S., Barnes, C. E., & Xue, Z. L. (1999). Investigation of uranyl adsorption on mesoporous titanium-based sorbents. Radiochim. Acta. 84, 37-42.

NUCLEAR MATERIALS

Actinide (Heavy Element) Chemistry

Project: 59967

Title: Aqueous Electrochemical Mechanisms in Actinide Residue Processing

PI: Dr. David E. Morris *Institution:* Los Alamos National Laboratory

Publication Type: Presentation

Morris, D. E. (1998, Jul. 27-30). Aqueous electrochemical mechanisms in actinide residue processing. DOE Environmental Management Science Program Workshop. Chicago, IL.

Morris, D. E. (1999, Apr. 21-25). Trends in actinyl electrochemistry: Voltammetry and theory. Presentation at the 217th National Meeting of the American Chemical Society. Anaheim, CA.

Morris, D. E. (1999, Aug. 22-26). Aqueous electrochemical mechanisms in mediated dissolution of actinide residues. First Accomplishments of Environmental Management Science Program. National Meeting of the American Chemical Society. New Orleans, LA.

Morris, D. E. (1999, Aug. 22-26). Aqueous electrochemical mechanisms in actinide residue processing results. Presentation at the National Meeting of the American Chemical Society. New Orleans, LA.

Engineering Science

Project: 60077

Title: Development of Nuclear Analysis Capabilities for DOE Waste Management Activities

PI: Dr. Cecil V. Parks *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

DeHart, M. D. (1998, Jun.). An advanced deterministic method for spent-fuel criticality safety analysis. Trans. Am. Nucl. Soc., 78, 170-172.

DeHart, M. D. (1999). A deterministic study of deficiencies in the Wigner-Seitz cell approximation. Trans. Am. Nucl. Soc., 80, 149-151.

Publication Type: Paper

Rearden, B. T. (2000, May 7-12). SAMS: A sensitivity analysis module for critically safety analysis using Monte Carlo techniques. Proceeds of PHYSOR 2000, ANS Int. Topical Meeting on Advances in Reactor Physics and Mathematics and Computation into the Next Millenium, CD-ROM, Pittsburgh, PA.

Publication Type: Presentation

Rearden, B. T. & Childs, R. L. (2000, Nov. 12-16). Prototypic sensitivity and uncertainty analysis codes for criticality safety with the SCALE code system. ANS/ENS 2000 International Winter Meeting and Embedded Topical Meetings. Washington, D. C. Trans. Am. Nucl. Soc. 83, 98-99.

Rearden, B. T., Hopper, C. M., Elam, K. R., Broadhead, B. L., & Fox, P. B. (2000, Nov. 12-16). Prototypic sensitivity and uncertainty analysis for experiment needs. ANS/ENS 2000 International Winter Meeting and Embedded Topical Meetings. Washington, D. C. Trans. Am. Nucl. Soc., 83, 103-106.

Rearden, B. T., Petrie, L. M., & Hollenbach, D. F. (2000, Oct. 23-26). Sensitivity and uncertainty analysis for nuclear criticality safety using keno in the scale code system. MC2000, International Conference on Advanced Monte Carlo for Radiation Physics, Particle Transport Simulation and Applications.

Publication Type: Proceeding

Broadhead, B. L., Childs, R. L., & Rearden, B. T. (1999, Sept. 20-24). Computational methods for sensitivity and uncertainty analysis in criticality safety. Proceedings of ICNC'99, Sixth International Conference on Nuclear Criticality Safety. Palais des Congres, Versailles, France. I, 57-65.

DeHart, M. D. (1999, Sept. 27-30). A deterministic study of the deficiency of the Wigner-Seitz approximation for Pu/MOX fuel pins. Proceedings of M&C '99 - Madrid, Mathematics and Computations Meeting. 689-699. Madrid, Spain.

Publication Type: Report

Parks, C. V., DeHart, M. D., Broadhead, B. L., Hopper, C. M., & Petrie, L. M. (1998, Jun.). Development of nuclear analysis capabilities for DOE waste management activities. Annual EMSP Summary Progress Report. ORNL/M-6549.

Parks, C. V., et. al. (1999, Jun.). Development of nuclear analysis capabilities for DOE waste management activities. Annual EMSP Summary Progress Report. ORNL/TM-1999/101.

Parks, C. V., et. al. (2000, Feb.). Development of nuclear analysis capabilities for DOE waste management activities. Annual EMSP Project Summary Report. ORNL/TM-2000/65.

Publication Type: Theses/Dissertations

Rearden, B. T. (1999). Development of SAMS: A three-dimensional sensitivity analysis module for the SCALE code system. PhD dissertation at Texas A&M University.

Materials Science

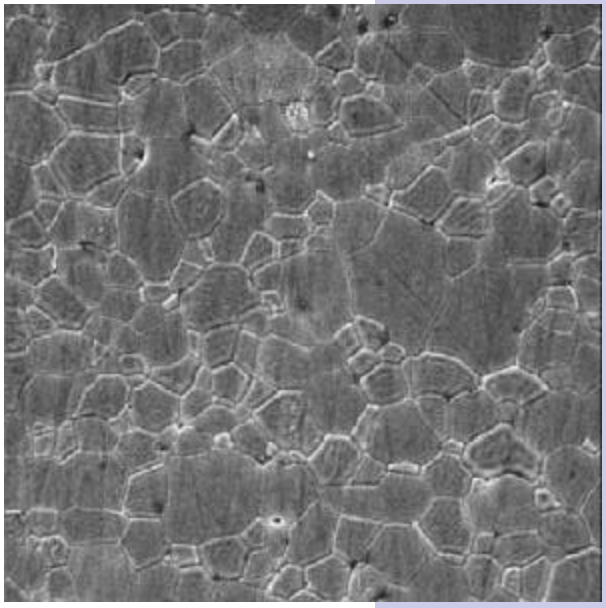
Project: 55094

Title: Chemical and Ceramic Methods Toward Safe Storage of Actinides Using Monazite
PI: Dr. P. E. D. Morgan
Institution: Rockwell International Corporation

Publication Type: Journal

Liu, G. K., Beitz, J. V., Huang, J., Abraham, M. M., & Boatner, L. A. (1997). Characterization of crystal field and nuclear quadrupole interactions in the 5D1 state of 243Am3+ in LaCl3 and CaWO4. Journal of Alloys and Compounds. 250, 347-351.

Liu, G. K., et. al. (1998). Crystal-field splitting, magnetic interaction, and vibronic excitations of 244Cm3+ in YPO4 and LuPO4. Journal of Chemical Phys. 109, 6800-6808.



Fully Dense, Stoichiometric La-Monazite, $LaPO_4$, ceramic, sintered to 1400?C - grain size ~2ìm. [see Project #55094]

Meldrum, A., Boatner, L. A., & Ewing, R. C. (1997). Electron-irradiation-induced nucleation and growth in amorphous LaPO4 and ScPO4, and zircon. Journal of Materials Research. 12, 1816.

Meldrum, A., Boatner, L. A., & Ewing, R. C. (1997). Displacive radiation effects in the monazite- and zircon-structure orthophosphates. Phys. Rev. B. 56, 13805.

Meldrum, A., Boatner, L. A., & Ewing, R. C. (1998). Effects of ionizing and displacive irradiation on several perovskite-structure oxides. Nuclear Instruments & Methods in Physics Research, Section B: Beam Interactions with Materials and Atoms. Elsevier Sci B. 141(347-352), 0168-583X.

Meldrum, A., Boatner, L. A., & Ewing, R. C. (1998). Phase transitions during ion-beam irradiation of the Perovskite-structure oxides. Ma, E., Bellon, P., Atmon, M., & Trivedi, R. (Eds.). Phase Transformation and Systems Driven far from Equilibrium. Materials Research Symposium Proceedings. 481, 401-406. Boston, MA.

Meldrum, A., Boatner, L. A., & Ewing, R. C. (2000, Apr.). A comparison of radiation effects in crystalline ABO sub-4-type phosphates and silicates. Mineral. Mag. 64(2), 185-194.

Meldrum, A., Boatner, L. A., & Zinkle, S. J. (1999). Effects of dose rate and temperature on the crystalline-to-metamict transformation in the ABO sub-4 Orthosilicates. Canadian Mineralogist. 37, 207-221.

Meldrum, A., Boatner, L. A., Wang, L. M., & Ewing, R. C. (1997). Ion-beam-induced amorphization of LaPO4 and ScPO4. Nuclear Instrum. Methods Phys. Res. B. 127/128, 160.

Meldrum, A., Boatner, L. A., Weber, W. J., & Ewing, R. C. (1998). Radiation damage in zircon and monazite. Geochim. Cosmochim. Acta. 62, 2509-2520.

Meldrum, A., Zinkle, S. J., Boatner, L. A., & Ewing, R. C. (1999). Heavy-ion irradiation effects in the ABO4 orthosilicates: Decomposition, amorphization, and recrystallization. Physical Review B. 59, 3981-3992.

Meldrum, A., Zinkle, S. J., Boatner, L. A., & Ewing, R. C. (1998). A transient liquid-like phase in the displacement cascades of zircon, hafnon, and thorite. Nature. 395, 56-58.

Nipko, J. C., et. al. (1997). Lattice dynamics of LuPO4. Journal of Alloys and Compounds. 250, 573.

Nipko, J. C., et. al. (1997). Lattice dynamics of xenotime: The phonon dispersion relations and density of states of LuPO4. Phys. Rev. B. 56, 11584.

Rapaport, A., David, V., Bass, M., Deka, C., & Boatner, L. A. (1999, Dec.). Optical spectroscopy of erbium-doped lutetium orthophosphate. J. Lumin. 85(1-3), 155-161.

Rapaport, A., Moteau, O., Bass, M., Boatner, L. A., & Deka, C. (1999). Optical spectroscopy and lasing properties of neodymium-doped lutetium orthophosphate. Jornal of Optical Soc. Am. B. 16, 911-916.

Publication Type: Presentation

Boatner, L. A. (1998, Mar. 5). Living in a materials world. Invited presentation for the induction seminar at the Academy of Sciences of Mexico. Mexico City, Mexico.

Boatner, L. A., Meldrum, A., Chakoumakos, B. C., & Mitchell, M. J. (1998, Sept. 11-12). The lanthanide orthophosphates: Chemically durable, radiation-resistant, high-temperature ceramics. Invited presentation at the Workshop on Advanced Materials for Extreme Environments: New Experimental Opportunities in Neutron Scattering. Argonne, IL.

Hanchar, J. M., Boatner, L. A., & Townsend, P. D. (1999, Apr. 25-28). Cathodoluminescence spectroscopy of the trivalent rare Earth elements in synthetic REEPO4, YPO4, and ScPO4. Presented at the American Ceramic Society 101st Annual Meeting. Indianapolis, IN.

Liu, G. K., et. al. (1997, Sep. 28 - Oct. 3). Self-radiation induced anisotropic structure damage in 244Cm-doped orthophosphate LuPO4. Presented at the 21st International Symposium on the Scientific Basis for Nuclear Waste Management, Davos Congress Center. Davos, Switzerland.

Loong, C. -K., Boatner, L. A., & Wang, J. Y. (1999, Jun. 20-23). Magnetic and thermodynamic properties of rare-Earth orthophosphates and pentaphosphates. Presentation at the 15th University Conference on Glass Science, University of Missouri. Rolla, MO.

Meldrum, A., Boatner, L. A., & Ewing, R. C. (1997, Dec. 1-5). Heavy-ion-irradiation of barium and strontium titanate: The effects of thermally-induced phase transitions and irradiation temperature. Presented at the Fall Meeting of the Materials Research Society, Symposium B: Phase Transformations and Systems Driven Far From Equilibrium. Boston, MA.

Meldrum, A., Boatner, L. A., & Ewing, R. C. (1999, Apr. 25-28). Radiation effects in Lanthanide-bearing AB04 compounds proposed for nuclear waste disposal. Presentation at a special focused session on Lanthanide-Containing Materials and Applications at the American Ceramic Society 101st Annual Meeting. Indianapolis, IN.

Meldrum, A., Boatner, L. A., Zinkle, S. J., & Ewing, R. C. (1999, Mar. 28 - Apr. 1). Ion irradiation effects in the zircon-structure orthosilicates. Presented at the 10th European Union of Geosciences. Strasbourg, France.

Meldrum, A., et. al. (1998, Nov. 30 - Dec. 4). Radiation effects in nonmetals: Amorphization, phase decomposition, and nanoparticles. Invited presentation at the 1998 Fall Materials Research Society Meeting. Boston, MA.

Meldrum, A., Ewing, R. C., & Boatner, L. A. (1997, Sep. 14-19). Effects of displacive and ionizing radiation on several perovskite-structure compounds. Presented at Radiation Effects in Insulators-9 (REI-9). Knoxville, TN.

Meldrum, A., Zinkle, S. J., Boatner, L. A., & Ewing, R. C. (1998, Aug. 31 - Sep. 4). Evidence for thermal spikes and cascade quenching in the zircon-structure orthosilicates. Presented at the Ion Beam Modification of Materials-98. Amsterdam, Netherlands.

Sales, B. C., Boatner, L. A., & Ramey, J. O. (1999, Jun. 20-23). Chromatographic studies of the structures of amorphous phosphates: A review. Presentation at the 15th University Conference on Glass Science, University of Missouri. Rolla, MO.

Trukhin, A. N. & Boatner, L. A. (1999, Aug. 16-20). Luminescence properties of ScPO4 single crystals. The 5th International Conference on Inorganic Scintillators and Their Applications, SCINT99, Moscow, Russia.

Weber, W. J., et. al. (1998, Nov. 30 - Dec. 4). The effect of temperature and recoil spectra on amorphization in zircon. Presented at the Fall Meeting of the Materials Research Society, Symposium N: Microstructural Processes in Irradiated Materials. Boston, MA.

Weber, W. J., et. al. (1999, Aug. 23-25). Ion-beam-induced defects and defect interactions in perovskite-structure titanates. Defects and Surface-Induced Effects in Advanced Perovskites. NATO Advanced Research Workshop. Jurmala, Latvia.

Publication Type: Proceeding

Devanathan, R., Weber, W. J., & Boatner, L. A. (1998). Response of zircon to electron and Ne+ irradiation. Ma, E., Bellon, P., Atmon, M., & Trivedi, R. (Eds.). Phase Transformation and Systems Driven far from Equilibrium. Materials Research Symposium Proceedings. 481, 419-424. Boston, MA.

Meldrum, A., Boatner, L. A., & Ewing, R. C. (1997). Electron-irradiation-induced crystallization of amorphous orthophosphates. Diaz de la Rubia, T., Was, G. S., Robertson, I. M., & Hobbs, L. W. (Eds.). Microstructure Evolution During Irradiation. Materials Research Society Symposium Proceedings. 439, 697-702.

Meldrum, A., Boatner, L. A., White, C. W., & Henderson, D. O. (1999). Radiation effects in nonmetals: Amorphization, phase decomposition, and nanoparticles. Ewing, R. C., Lucas, G., Williams, J., & Zinkle, S. (Eds.). Microstructural Processes in Irradiated Materials. Materials Research Symposium Proceedings. 540, 135. Boston, MA.

Meldrum, A., et. al. (1999). Radiation effects in zircon, hafnon, and thorite: Implications for Pu disposal. Ewing, R. C., Lucas, G., Williams, J., & Zinkle, S. (Eds.). Microstructural Processes in Irradiated Materials. Materials Research Symposium Proceedings. 540, 395. Boston, MA.

Weber, W. J., et. al. (1999). The effect of temperature and damage energy on amorphization in zircon. Ewing, R. C., Lucas, G., Williams, J., & Zinkle, S. (Eds.). Microstructural Processes in Irradiated Materials. Materials Research Symposium Proceedings. 540,367. Boston, MA.

Publication Type: Theses/Dissertations

Meldrum, A. (1999). Radiation effects in the orthophosphates. PhD dissertation at the Department of Earth Sciences, University of New Mexico. Albuquerque, NM.

Project: 55382

Title: Determination of Transmutation Effects in Crystalline Waste Forms
PI: Dr. Don Reed *Institution:* Argonne National Laboratory

Publication Type: Journal

Fortner, J. A., Buck, E. C., Strachan, D. M., & Hess, N. J. (1998). Extended electron loss fine structure analysis of silicon-K edges using an imaging filter. Microscopy & Microanalysis. 4 (Suppl. 2: Proceedings):706-707.

Hess, N. J., Balmer, M. L., Conradson, S. D., & Bunker, B. C. (1997). Ti XAS of a novel Cs-silicotitanate. Journal of Solid State Chemistry, 129:206-213.

Publication Type: Proceeding

Hess, N. J., et. al. (1997). Characterization of electroactive Cs ion-exchange materials using XAS. Materials Research Society Proceedings. 456:813-818.

Project: 60118

Title: Fundamental Thermodynamics of Actinide-Bearing Mineral Waste Forms
PI: Dr. Mark A. Williamson
Institution: Argonne National Laboratory

Publication Type: Journal

Putnam, R. L., Navrotsky, A., Cordfunke, E. H. P., Huntelaar, M. E., & Woodfield, B. F. (1999, Feb.). Thermodynamics of formation for zirconolite (CaZrTi2O7) from T= 298.15K to T=1500K. J. Chem. Thermodyn. 31(2), 229-243.

High temperature solution calorimeter at Los Alamos National Laboratory. This calorimeter is the same type used in studies of non-radioactive materials but has been installed in a section of the laboratory to allow the use of Pu-bearing samples to measure the formation energetics of Pu-bearing materials. A 1997 DOE EMSP grant helped establish the facility and will support the measurement of Pu-bearing waste ceramics being synthesized at LLNL. [see Project #60118]

Putnam, R. L., Navrotsky, A., Woodfield, B. F., & Boerio-Goates, J. (1999). Heat capacity, third law entropy, and formation energetics of zirconolite, CaZrTi2O7. Environmental Issues and Waste Management Technologies in the Ceramic and Nuclear Industries IV, Ceramic Transactions. 93, 339.

Putnam, R. L., Navrotsky, A., Woodfield, B. F., Boerio-Goates, J., & Shapiro, J. L. (1999). Thermodynamics of formation of zirconolite (CaZrTi2O7) from T = 298.15 K to T = 1500 K. J. Chem. Thermo. 31(3), 229-243.

Putnam, R. L., Navrotsky, A., Woodfield, B. F., Shapiro, J. L., & Boerio-Goates, J. (1999). Heat capacity, third law entropy, and formation energetics of zirconolite, CaZrTi2O7. Marra, J. C. & Chandler, G. T. (Eds.), Environmental Issues and Waste Management Technologies in the Ceramic and Nuclear Industries IV, Ceramic Transactions, 93. The American Ceramic Society. Westerville, OH.

Woodfield, B. F., Boerio-Goates, J., Shapiro, J. L., Putnam, R. L., & Navrotsky, A. (1999). Molar heat capacity and thermodynamic functions of zirconolite, CaZrTi2O7. J. Chem. Thermo. 31(3), 245-253.

Woodfield, B. F., et. al. (1999, Dec.). Molar heat capacity and thermodynamic functions for CaTiO3. J. Chem. Thermodyn. 31(12), 1573-1583.

Publication Type: Other

Putnam, R. L., Ph.D. Dissertation. (1999, Nov.). Department of Geosciences, Princeton University, NJ.

Publication Type: Presentation

Putnam, R. L., et. al., (1998, Dec.). Thermochemistry of Hf-zirconolite, CaHfTi2O7. Scientific Basis for Nuclear Waste Management, Materials Research Society.

Publication Type: Proceeding

Putnam, R. L., et. al. (1999, in press). Thermochemistry of Hf-zirconolite, CaHfTi2O7. MRS Proceedings.

Project: 60387

Title: Distribution & Solubility of Radionuclides & Neutron Absorbers in Waste Forms for Disposition of Plutonium Ash & Scraps, Excess Plutonium, and Misc. Spent Nuclear Fuels

PI: Dr. Denis M. Strachan *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Gu, B. X., Wang, L. M., & Ewing, R. C. (2000, Mar.). The effect of amorphization on the Cs ion exchange and retention capacity of zeolite-NaY. J. Nucl. Mater. 278(1), 64-72.

Li, L. Y., et. al. (2000, Jul.). Crystallization of gadolinium- and lanthanum-containing phases from sodium alumino-borosilicate glasses. J. Non-Cryst. Solids. 272(1), 46-56.

Li, L., Strachan, D. M., Li, H., Davis, L. L., & Qian, M. (1999, in press). Peraluminous and peralkaline effects on Gd2O3 and La2O3 solubilities in sodium-alumino-borosilicate glasses. Ceramic Transactions. American Ceramic Society. Westerville, OH.

Zhao, D., et. al. (1999, in press). Electron microprobe and electron microscopy characterization of precipitated gadolinium crystals in borosilicate glasses. Journal of Non-Crystalline Solids.

Publication Type: Other

Feng, X., et. al. (1999). Distribution and solubility of radionuclides in waste forms for disposition of plutonium and spent nuclear fuels: Preliminary results. Marra, J. C. & Chandler, G. T. (Eds.), Ceramic Transactions. 93, 409-419. American Ceramic Society, Westerville, OH.

Publication Type: Presentation

Davis, L. L., et. al. (1998, Dec.). The effects of Na2O, Al2O3, and B2O3 on HfO2 solubility in borosilicate glass. Materials Research Society, Boston, MA.

Feng, X. (1998, Mar. 17). A plasma arc-vitreous ceramic process for stabilizing EBR-II spent nuclear fuels. National Academy of Science.

Feng, X., et. al. (1998, May). Distribution and solubility of radionuclides in waste forms for disposition of plutonium and spent nuclear fuels: Preliminary results. Symposium of Waste Management Science and Technology in the Ceramic and Nuclear Industries. 100th Am. Cer. Soc. Annual Meeting. Cincinnati, OH.

Li, L., Strachan, D. M., Davis, L. L., Li, H., & Qian, M. (1998, Dec.). Gadolinium solubility limits in sodium-alumino-borosilicate glasses. Materials Research Society Meeting. Boston, MA.

Li, L., Strachan, D. M., Li, H., Davis, L. L., & Qian, M. (1999, Apr. 24-29). Peraluminous and peralkaline effects on Gd2O3 and La2O3 solubilities in sodium-alumino-borosilicate glasses. American Ceramic Society Meeting. Indianapolis, IN.

Shuh, D. K., et. al. (1998, Jul. 28). Distribution and solubility of radionuclides and neutron absorbers in forms for disposition of plutonium ash and scraps, excess plutonium, and miscellaneous spent nuclear fuels. Environmental Management Science Program Workshop Plenary Address. Chicago, IL.

Shuh, D. K., et. al. (1998, Jul. 9). Investigations of actinide materials chemistry utilizing synchrotron radiation methods. Chemical and Analytical Sciences Division, Oak Ridge National Laboratory. Oak Ridge, TN.

Stachan, D. M. (1999, Jun. 1). The Yucca Mountain repository: What has changed? American Geophysical Union, Spring Meeting. Boston, MA.

Strachan, D. M. (1999, Apr. 22). Radiation effects in ABO4 orthophosphates and orthosilicates. Invited presentation at theHLW and Pu Immobilization Workshop. CEA, Saclay, France.

Strachan, D. M. (1999, Apr. 5). Performance assessments: The design, selection and importance of nuclear waste forms. Invited presentation at Ch Performance Assessments: The Design, Selection and Importance of Nuclear Waste Forms.

Strachan, D. M. (1999, Jul. 12). Ageing studies of nuclear waste forms: The evaluation of long-term behaviour. Plenary lecture for International Conference on Ageing Studies & Lifetime Extension of Materials, St. Catherine's College. Oxford, United Kingdom.

Strachan, D. M. (1999, Oct. 20). Natural systems: Applications to nuclear waste management. Invited presentation at workshop sponsored by the Russian Academy of Sciences and the U.S. Department of Energy. Moscow, Russia.

Strachan, D. M. (1999, Sept. 10). Radiation effects in zircon. Invited seminar at the Université Henri Poincaré. Nancy, France.

Vance, E. R., et. al. (1999, Apr. 28). Crystal chemistry, radiation effects and aqueous leaching of brannerite, UTi2O6. S-I-059-99, Materials Division, ANSTO, Menai, NSW 2234, Australia.

Publication Type: Proceeding

Davis, L. L., et. al. (1998). The effects of Na2O, Al2O3, and B2O3 on HfO2 solubility in borosilicate glass. In Scientific Basis for Nuclear Waste Management XXII. Materials Research Society. Pittsburgh, PA.

Ewing, R. C. (1999, in press). Ageing studies of nuclear waste forms: The evaluation of long-term behaviour. Proceedings of International Conference on Ageing Studies & Lifetime Extension of Materials.

Li, L., Strachan, D. M., Davis, L. L., Li, H., & Qian, M. (1998). Gadolinium solubility limits in sodium-alumino-borosilicate glasses. In Scientific Basis for Nuclear Waste Management XXII, Materials Research Society. Pittsburgh, PA.

Strachan, D. M. (1999, Nov. 13). Mineralogy: Applications to nuclear waste disposal. Plenary presentation at the Twentieth Annual New Mexico Mineral Symposium, New Mexico Institute of Mining and Technology. Socorro, NM.

Wang, S. X., Wang, L. M., & Ewing, R. C. (1999). Electron irradiation of zeolites. In Zinkle, S. J., Lucas, G. E., Ewing, R. C., & Williams, J. S. (Eds.), Microstructural Processes in Irradiated Materials. Symposium Proceedings of the Materials Research Society. 540, 361-366.

SPENT NUCLEAR FUEL

Engineering Science

Project: 60144

Title: Flow Visualization of Forced and Natural Convection in Internal Cavities
PI: Dr. John C. Crepeau *Institution:* University of Idaho

Publication Type: Journal

Condie, K. G., Stoots, C. M., McEligot, D. M., Becker, S., & Durst, F. (1998). Measurements of induced boundary layer transition in the new INEEL Matched-Index-of-Refraction flow system. American Physical Society Fluid Dynamics Meeting. Bulletin APS. 43, 2092.

Nishimura, M., Fujii, S., Shehata, A. M., Kunugi, T., & McEligot, D. M. (1997). Prediction of forced gas flows in circular tubes at high heat fluxes. NuReTH-8, Kyoto.

Shehata, A. M. & McEligot, D. M. (1998). Mean structure in the viscous layer of stongly-heated internal gas flows. International Journal of Heat Mass Transfer. 41, 4297-4313.

Publication Type: Presentation

Crepeau, J. C. (2000, Sep. 13). Drying of spent nuclear fuel. Presentation for the Mechanical Engineering Department of the University of Idaho Extension, Idaho Falls, ID.

Ezato, K., Shehata, A. M., Kunugi, T., & McEligot, D. M. (1997). Numerical predictions of transitional features of turbulent forced gas flows in circular tubes with strong heating. ASME Fluids Engineering Conference. Vancouver, British Columbia, Canada.

McEligot, D. M. (1997). Maximum allowable heat flux for a submerged tube bundle. Engineering Conference on Convective Flow and Pool Boiling. Irsee, Germany.

McEligot, D. M., Shehata, A. M., & Kunugi, T. (1998). Prediction of strongly-heated gas flows. Invited presentation at the Engineering Foundation Conference on Turbulent Heat Transfer II, I. 33-47. Manchester, U. K.

Publication Type: Proceeding

Crepeau, J. C., et. al. (1998, Sept.). Fluid mechanic studies relating to drying and passivation in an idealized SNF cannister. ANS 3rd Topical Meeting on Spent Nuclear Fuel and Fissile Material Management. Charleston, SC.

McCreery, G. E. & Martineau, R. M. (1998, Nov.). An experimental investigation of steam injection in fractured porous media. ASME International Mechanical Engineering Congress. Anaheim, CA.

McCreery, G. E., et. al. (1999, Sept. 6-9). Flow visualization and velocity measurements in a model fuel storage canister. ANS Global '99 International Conference on Future Nuclear Systems. Jackson, WY.

McCreery, G. E., Kullberg, C. M., Schultz, R. R., Yonomoto, T., & Anoda, Y. (1997). Heat transfer modeling of the LSTF Passive Residual Heat Removal System. ASME Nuclear Engineering Division, ASME Symposium of the 1997 International Mechanical Engineering Congress. Dallas, TX. 97-106.

Geochemistry

Project: 59849

Title: Radionuclide Immobilization in the Phases Formed by Corrosion of Spent Nuclear Fuel: The Long-Term Assessment

PI: Dr. Rodney C. Ewing *Institution:* University of Michigan

Publication Type: Paper

Jensen, K. A. & Ewing, R. C. (2000). The Okelobondo natural fission reactor, southeast Gabon: Geology, mineralogy, and retardation of nuclear-reaction products. Geological Society of America Bulletin. 113(1), 32-62.

Project: 73691 (Renewal of Project No. 59960)

Title: Renewal of Direct Investigations of the Immobilization of Radionuclides in the Alteration Products of Spent Nuclear Fuel

PI: Dr. Peter C. Burns *Institution:* University of Notre Dame

Publication Type: Journal

Burns, P. C. & Finch, R.J. (1999, Sep.). Wyartite: Crystallographic evidence for the first pentavalent-uranium mineral. Am. Mineral. 84(9), 1456-1460.

Burns, P. C. & Hill, F. C. (2000, Feb.). A new uranyl sheet in K-5[(UO2)(10)O-8(OH)(9)](H2O): New insight into sheet anion-topologies. Can. Mineral. 38, 163-173, Part 1.

Burns, P. C. & Hill, F. C. (2000, Feb.). Implications of the synthesis and structure of the Sr analogue of curite. Can. Mineral. 38, 175-181, Part 1.

Burns, P. C. (1998). The structure of boltwoodite and implications of solid-solution towards sodium boltwoodite. Canadian Mineralogist. 36, 1069-1075.

Burns, P. C. (1998). The structure of compreignacite, K2[(UO2)3O2(OH)3]2(H2O)7. Canadian Mineralogist. 36, 1061-1067.

Burns, P. C. (1999. Cs boltwoodite obtained by ion exchange from single crystals: Implications for radionuclide release in a nuclear repository. J. Nucl. Mater. 265, 218-223.

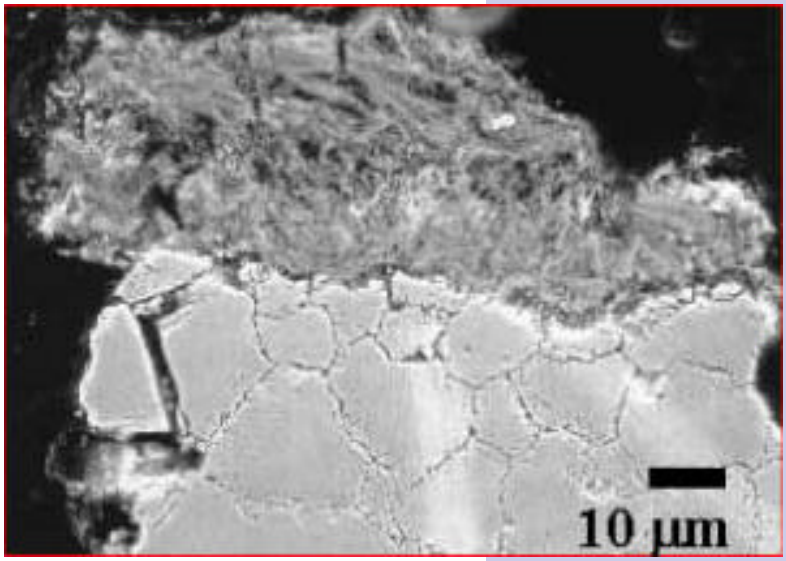
Burns, P. C., Olson, R. A., Finch, R. J., Hanchar, J. M., & Thibault, Y. (1999). KNa3(UO2)2(Si4O10)2(H2O)(4), a new compound formed during vapor hydration of an actinide-bearing borosilicate waste glass. J. Nucl. Mater. 278(2-3), 290-300.

Burns, P.C. (2000, May-Jun.). A new uranyl phosphate chain in the structure of parsonsite. Am. Mineral. 85(5-6), 801-805.

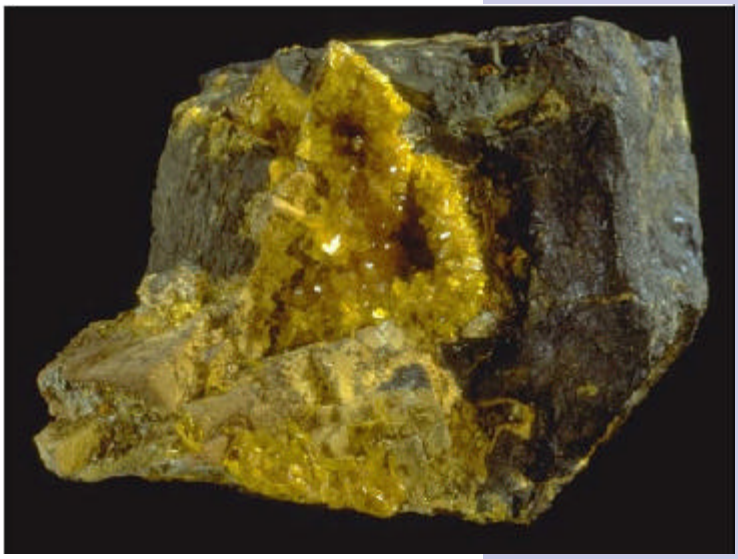
Chen, F. R., Burns, P. C., & Ewing, R. C. (2000, Apr.). Near-field behavior of Tc-99 during the oxidative alteration of spent nuclear fuel. J. Nucl. Mater. 278(2-3), 225-232.

Chen, F., Burns, P. C., & Ewing, R. C. (1999, Oct.). Se-79: Geochemical and crystallo-chemical retardation mechanisms. J. Nucl. Mater. 275(1), 81-94.

Hill, F.C. & Burns, P.C. (1999, Oct.). The structure of a synthetic Cs uranyl oxide hydrate and its relationship to compreignacite. Can. Mineral. 37, 1283-1288, Part 5.



Laboratory Studies: Argonne National Labs
High Drip Rate Tests:
Alteration Phases:
Boltwoodite: (K,Na)[(UO2)(SiO3OH)](H2O)1.5
Uranophane: Ca[(UO2)(SiO3OH)]2(H2O)5
[see Project #73691, renewal of #59960]



The mineral uraninite, UO2, is an excellent natural analogue for UO2 (LWR) spent fuel. This photograph shows a specimen of uraninite (black) that has been oxidized under conditions broadly similar to those that will be present in the proposed repository at Yucca Mountain. The uranyl phases that have formed due to the alteration (oxidation) are clearly visible as yellow and orange crystals. We obtain many of the crystals used in our studies from similar natural occurrences. These minerals are typically identical to the phases that form when spent fuel is corroded during laboratory tests at ANL. [see Project #73691, renewal of #59960]

Publication Type: Paper

Burns, P. C. (1999, in press). The crystal chemistry of uranium. Mineralogical Society of America Reviews in Mineralogy.

Publication Type: Presentation

Burns, P. C. & Finch, R. J. (1999). The structure of wyartite: Crystallographic evidence for the first pentavalent-uranium mineral. GAC-MAC. Sudbury, Ontario, Canada.

Burns, P. C. (1998): Topological aspects of uranyl mineral structures. IMA. Toronto, Canada.

Burns, P. C., Finch, R. C. & Wronkiewicz, D. J. (1998). Direct investigations of the immobilization of radionuclides in the alteration products of spent nuclear fuel. DOE Environmental Management Science Program Workshop. Chicago, IL.

Hill, F. C. & Burns, P. C. (1998). Chemical and structural diversity in the uranyl oxide hydrate system. GSA Toronto, Canada.

Hill, F. C. & Burns, P. C. (1998). Investigations of the crystal chemistry of uranyl oxide hydrates. IMA Toronto, Canada.

Hill, F. C. & Burns, P. C. (1999). The importance of uranyl silicates for the disposal of nuclear waste. GAC-MAC. Sudbury, Ontario, Canada.

Kim, C. W. & Wronkiewicz, D. J. (1998). Alteration phases of spent nuclear fuel. Missouri Academy of Sciences, 1998 Annual Meeting.

Publication Type: Proceeding

Chen, F., Burns, P.C., & Ewing, R.C. (1998, in press). 79-Se: Geochemical and crystallo-chemical retardation mechanisms. The Scientific Basis for Nuclear Waste Management XX. MRS Proceedings.

Project: 73751 (Renewal of Project No. 59849)

Title: Corrosion of Spent Nuclear Fuel: The Long Term Assessment
PI: Dr. Rodney C. Ewing *Institution:* University of Michigan

Publication Type: Journal

Casas, I., et. al. (1998). The role of pe, pH, and carbonate on the solubility of UO2 and uraninite under nominally reducing conditions. Geochimica et Cosmochimica Acta. 62(13), 2223-2231.

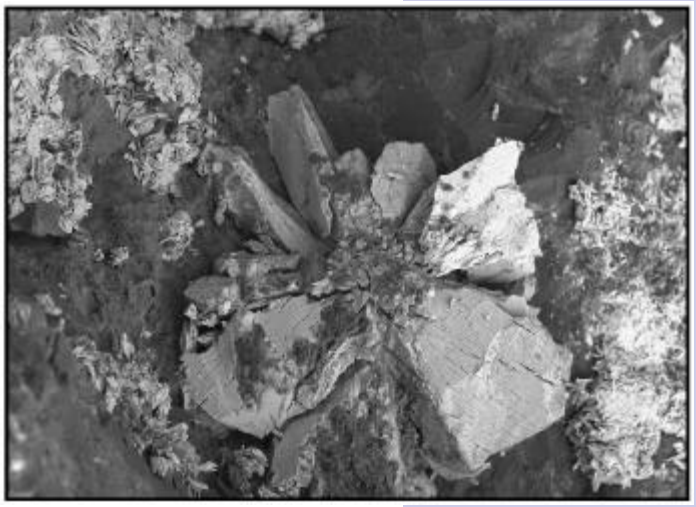
Chen, F. & Ewing, R. C. (1999, in press). Structural contributions to the third-law entropies of uranyl phases. Geochimica et Cosmochimica Acta.

Chen, F., Burns, P. C., & Ewing, R. C. (1999). 79-Se: Geochemical and crystallo-chemical retardation mechanisms. J. Nucl. Mater. 275, 81-94.

Chen, F., Burns, P. C., & Ewing, R. C. (1999, in press). Near-field behavior of 99-Tc during the oxidative alteration of spent nuclear fuel. J. Nucl. Mater.

Chen, F., Ewing, R. C., & Clark, S. B. (1999). The Gibbs free energies and enthalpies of formation of uranium (VI) phases: An empirical method of prediction. American Mineralogist. 84(4), 650-654.

Clark, S. B., Ewing, R. C., & Schaumloffel, J. C. (1998). A method to predict free energies of formation of mineral phases in the U(VI)-SiO2-H2O system. Journal of Alloys and Compunds. 271, 189-193.



SEM-image of a sandstone sample from a U-deposit open pit in Oklo-Okélobondo in Gabon of West-Central Africa, coated with aggregates of johanneite, uranyl sulfate hydroxide hydrate, silica, and kaolinite. [see Project #73751, renewal of #59849]

Ewing, R. C. (1999). Less geology in the geological disposal of nuclear waste. Science. 286, 415-416.

Ewing, R. C., Tierney, M. S., Konikow, L. F., & Rechard, R. P. (1999). Performance assessments of nuclear waste repositories: A dialogue on their value and limitaions. Risk Analysis. 19(5), 933-958.

Fayek, M., Burns, P., Guo, Y. -X., & Ewing, R. C. (2000). Micro-structures associated with uraninite alteration. J. Nucl. Mater. 277, 204-210.

Finch, R. J., Cooper, M. A., Hawthorne, F. C., & Ewing, R. C. (1999). Refinement of the crystal structure of rutherfordine. Canadian Mineralogist. 37, 929-938.

Finch, R. J., Hawthorne, F. C., & Ewing, R. C. (1998). Structural relations among schoepite, metaschoepite, and “dehydrated schopite.” Canadian Mineralogist. 36, 831-845.

Jensen, K. A. & Ewing, R. C. (1999, in press). The Okelobondo natural fission reactor, southeast Gabon: Geology, mineralogy, and retardation of nuclear reaction products. Geological Society of America Bulletin.

Zhao, D. & Ewing, R. C. (2000, in press). Alteration products of uraninite from the Colorado Pleateau. Radiochimica Acta.

Publication Type: Presentation

Ewing, R. C. (1999, Apr. 22). Radiation effects in AB04 orthophosphates and orthosilicates. Invited presentation at the HLW and Pu Immobilization Workshop, CEA. Saclay, France.

Ewing, R. C. (1999, Apr. 5). Performance assessments: The design, selection and importance of nuclear waste forms. Invited presentation at the Chemistry Division Colloquium, Argonne National Laboratory. Argonne, IL.

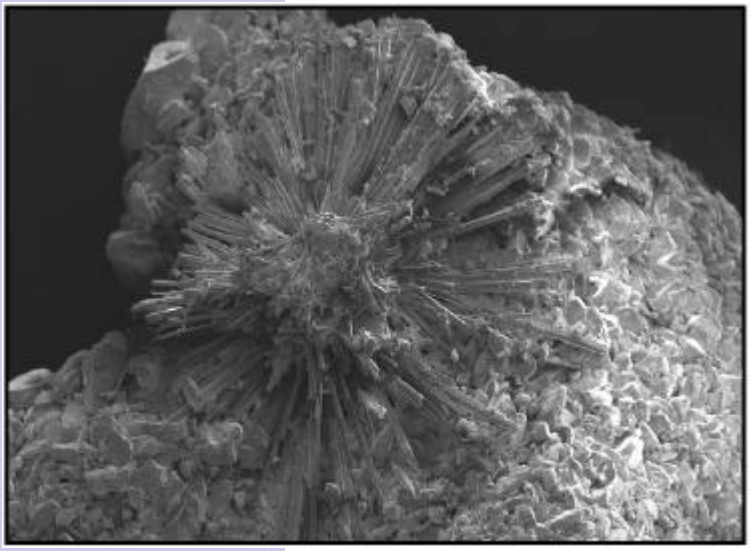
Ewing, R. C. (1999, Jul. 12). Ageing studies of nuclear waste forms: The evaluation of long-term behaviour. Plenary lecture at the International Conference on Ageing Studies & Lifetime Extension of Materials. St. Catherine's College. Oxford, United Kingdom.

Ewing, R. C. (1999, Jun. 1). The Yucca Mountain Repository: What has changed? Invited presentation at the American Geophysical Union, Spring Meeting. Boston, MA.

Ewing, R. C. (1999, Nov. 13). Mineralogy: Applications to nuclear waste disposal. Plenary presentation at the Twentieth Annual New Mexico Mineral Symposium. New Mexico Institute of Mining and Technology. Socorro, NM.

Ewing, R. C. (1999, Oct. 20). Natural systems: Applications to nuclear waste management. Invited presentation at a workshop sponsored by the Russian Academy of Sciences and the U. S. Department of Energy. Moscow, Russia.

Ewing, R. C. (1999, Sep. 10). Radiation effects in zircon. Invited seminar at the Universite Henri Poincare. Nancy, France.



SEM-image of johanneite with precipitates of acicular gypsum on a sandstone sample from the Oklo open pit. [see Project #73751, renewal of 59849]

Ewing, R. C. (1999, Sept. 26 - Oct. 1). Results of uranyl phase analyses. Presented at the Seventh International Conference on the Chemistry and Migration Behavior of Actinides and Fission Products in the Geosphere. Lake Tahoe, CA.

Publication Type: Proceeding

Chen, F. & Ewing, R. C. (1999). 79-Se: Geochemical and crystallochemical retardation mechanisms. Symposium Proceedings of the Materials Research Society. 556, 1115-1122.

Chen, F. & Ewing, R. C. (1999). Structural contributions to the third-law entropy of uranyl phases. Symposium Proceedings of the Materials Research Society. 556, 1017-1024.

Ewing, R. C. (1999). Nuclear waste forms for actinides. Proceedings of the National Academy of Sciences. 96(7), 3432-3439.

Separations Chemistry

Project: 60392

Title: Radiolytic and Thermal Process Relevant to Dry Storage of Spent Nuclear Fuels

PI: Dr. Steven C. Marschman *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Petrik, N. G., Alexandrov, A. B., Vall, A., & Orlando, T. M. (1999, in press). Gamma radiolysis of water on oxide surfaces: Parameters controlling the energy transfer.

Petrik, N. G., Taylor, D. P., & Orlando, T. M. (1999). Laser-stimulated luminescence of yttria-stabilized cubic-zirconia crystals. J. Appl. Phys. 85, 6770.

Simpson, W. C., Wang, W. K., Yarmoff, J. A., & Orlando, T. M. (1999). Photon- and electron-stimulated desorption of O + from zirconia. Surf. Sci. 423, 225.

Publication Type: Presentation

Haustein, P. (1999, Aug. 22-26). Nuclear stimulated desorption at the surfaces of model SNF materials: Experiment and computer simulation. Invited presentation at the Annual Symposium on First Accomplishments of the Environmental Management Science Program, American Chemical Society. New Orleans, LA.

Hedhili, M. N., Yakshinskiy, B. V., & Madey, T. E. (1999, Mar. 21-25). Interaction of water with UO2 (001). National American Physical Society Meeting. Atlanta, GA.

Hedhili, M. N., Yakshinskiy, B. V., Madey, T. E., Dobrozemsky, R., & Yarmoff, J. (1999, Aug. 22-26). Interaction of water with uranium oxide surfaces. Annual Symposium on First Accomplishments of the Environmental Management Science Program. American Chemical Society. New Orleans, LA.

Orlando, T. M. (1999, Mar. 21-25). Quantum-resolved studies of condensed phase reactions. Invited presentation at the Annual Meeting of the Symposium on Free radicals in the Condensed Phase. American Chemical Society. Anaheim, CA.

Orlando, T. M., Petrik, N. G., Alexandrov, A. B., & Simpson, W. C. (1999, Feb. 26). Nonthermal processes on oxide surfaces and interfaces. Invited presentation at the Department of Chemistry, University of Utah. Salt Lake City, UT.

Orlando, T. M., Petrik, N. G., Alexandrov, A. B., & Simpson, W. C. (1999, Feb. 24-25). Nonthermal processes on oxide surfaces and interfaces. DOE Laboratory Catalysis Research Symposium. Albuquerque, NM.

Orlando, T. M., Petrik, N. G., Alexandrov, A. B., & Simpson, W. C. (1999, Feb. 24). Nonthermal processes on oxide surfaces and interfaces. Invited presentation at the Los Alamos National Laboratory. Los Alamos, NM.

Orlando, T. M., Petrik, N., Marshman, S., & Camaioni, D. M. (1999, Nov. 14-18). Nonthermal surface processes in the generation of gas in mixed wastes. Invited presentation at the Annual Meeting of the American Nuclear Society. Long Beach, CA.

Petrik, N., Marshman, S., Camaioni, D. M., & Orlando, T. M. (1999, Aug. 22-26). Nonthermal surface and interface processes in the storage of spent nuclear fuel and mixed wastes. Annual Symposium on First Accomplishments of the Environmental Management Science Program. American Chemical Society. New Orleans, LA.

SUBSURFACE CONTAMINATION

Actinide (Heavy Element) Chemistry

Project: 70050

Title: Novel Optical Detection Schemes for In-Situ Mapping of Volatile Organochlorides in the Vadose Zone

PI: Dr. S. Michael Angel *Institution:* University of South Carolina

Prototype coaxial fiber/electrode REMPI probe. [see Project #70050]

Publication Type: Poster

Chinni, R. C., et. al. (2000, Sept.). Resonance-enhanced multiphoton ionization (REMPI) measurements using visible excitation and a compact intergrated fiber-optic probe. Federation of Analytical Chemistry and Spectroscopy Societies (FACSS). Nashville, TN.

Publication Type: Presentation

Angel, S. M., et. al. (2000, Nov. 28-30). In-situ resonance-enhanced multiphoton ionization (REMPI) measurements using a fiber-optic probe. FY2001 EMSP Vadose Zone Principal Investigator Workshop. Pacific Northwest National Laboratory. Richland, WA.

Angel, S. M., et. al. (2000, Oct. 12). In-situ resonance-enhanced multiphoton ionization (REMPI) measurements using a fiber optic probe. Invited plenary lecture at the The Tenth International Syposium on Resonance Ionization Spectroscopy & Its Applications (RIS-2000).

Chinni, R. C., et. Al. (2000, Sept.). Fiber-optic resonance-enhanced multiphoton ionization (REMPI) analyses of volatile organic compounds using visible excitation. Paper #SE06-03. The International Society for Optical Engineering (SPIE Opto Southeast). Charlotte, NC.

Chinni, R. C., et. al. (2001, Mar.). A miniature fiber-optic resonance-enhanced multiphoton ionization probe (REMPI) with no focusing optics. Paper #734, The Pittsburgh Conference & Exposition (PiitCon). New Orleans, LA.

Publication Type: Proceeding

Angel, S. M., et. al. (2000, Oct.). In-situ resonance-enhanced multiphoton ionization (REMPI) measurements using an optical fiber probe. Resonance Ionization Spectroscopy 2000. Proceedings of the Tenth International Symposium. Knoxville, TN.

Project: 70132 (Renewal of Project No. 54683)

Title: Speciation, Mobility and Fate of Actinides in the Groundwater at the Hanford Site

PI: Dr. Ken O. Buesseler *Institution:* Woods Hole Oceanographic Institute

Publication Type: Journal

Dai, M., et al. (1999, in press). Size fractionated Pu isotopes in a coastal environment. J. Enivronmental Radioactivity.

Yue, Y. K., Wang, J. J., & Dai, M. (2000, Jul. 25). Volumetric and fluorescence studies of aqueous solutions containing n-octylamine, cetyltrimethylammonium bromide, and salt. Langmuir. 16(15), 6114-6117.

Publication Type: Presentation

Buesseler, K. O., et. al. (1999, Nov. 16-18). Speciation, mobility, and fate of actinides in the groundwater at the Hanford Site. EMSP PI workshop.

Dai, M., et al. (1998, May). Size fractionated Pu isotopes in the ocean, a pond and groundwater. AGU Spring Meeting, Boston, MA. EOS. 79(17), 138.

Dai, M., et al. (1999, May). Isotopic composition, speciation and mobility of Pu in the groundwater at DOE Savannah River Site. AGU Spring meeting. Boston, MA.

Dai, M.H., et. al. (1998, July 27- 30). Size fractionated Pu isotopes in surface and subsurface waters. American Chemical Society DOE Environmental Management Science Program Workshop. Chicago, IL.

Repeta, D.J., Quan, T. M., Aluwihare, L. I., & Accardi, A. (1999). Dissolved organic matter in fresh and marine waters. Amer. Soc. Limnol. Oceanogr. Annual meeting. Santa Fe, NM.

Project: 70176

Title: Transuranic Interfacial Reaction Studies on Manganese Oxide Hydroxide Mineral Surfaces

PI: Dr. Heino Nitsche *Institution:* Lawrence Berkeley National Laboratory

Publication Type: Poster

Nitsche, H., Serne, R. J., Shaughnessy, D. A., Shuh, D. K., & Waychunas, G. A. (2000, Apr. 24-28). Transuranic interfacial reaction studies on manganese oxide hydroxide mineral surfaces. Environmental Management Science Program National Workshop, Atlanta, GA.

Shaughnessy, D. A., et. al. (2000, Aug. 20-24). Interfacial reaction studies of plutonium with manganese oxide hydroxide mineral surfaces (Abstract No. ENVR227). 220th National Meeting of the American Chemical Society, Washington, D. C.

Publication Type: Presentation

Nitsche, H. (2000, Apr. 24-28). Actinides and the environment: The challenge for interdisciplinary research (Abstract No. NUCL30). Chemical and Nuclear Properties of the Heaviest Elements: A Symposium in Memory of Glenn T. Seaborg, 220th National Meeting of the American Chemical Society, Washington D. C.

Project: 73819 (Renewal of Project No. 59996)

Title: Plutonium Speciation, Solubilization, and Migration in Soils

PI: Dr. Mary P. Neu *Institution:* Los Alamos National Laboratory

Publication Type: Presentation

Neu, M. P. (1999, Sep. 26-30). The migration behavior of collodial CE, Eu, Zr, and ionic Am and Np in selected solid-matrix materials. Presentation at Migration-99.

Neu, M. P. (1999, Sep. 26-30). Transport behavior of ionic and collodial forms of plutonium. Presentation at Migration-99.

Analytical Chemistry & Instrumentation

Project: 54639

Title: Development of an In-Situ Microsensor for the Measurements of Chromium and Uranium in Groundwater at DOE Sites

PI: Dr. Joseph Wang *Institution:* New Mexico State University

Publication Type: Journal

Daniele, S., Bragato, C., Baldo, M. A., Wang, J., & Lu, J. (2000, Apr.). The use of a remote stripping sensor for determination of copper and mercury in the Lagoon of Venice. Analyst. 125(4), 731-735.

Daniele, S., Bragato, C., Wang, J., & Lu, J. (2000). Remote stripping sensor for determining copper in the lagoon of Venice. 125, 731.

Wang, J. (1997). Remote electrochemical sensors. Trends Anal. Chem. 16, 84.

Wang, J. (2000). From remote sensors to submersible labs. Invited paper in Lab. Robotics and Automation. 12, 178.

Wang, J., Adeniyi, W., & Kounaves, S. (2000). Adsorptive stripping analysis of trace nickel at iridium-based ultramicroelectrode arrays. Electroanalysis. 12, 44.

Wang, J., Bhada, R., Lu, J., & MacDonald, D. (1998). Remote sensor for monitoring TNT in natural waters. Anal. Chim. Acta. 361, 85.

Wang, J., et. al. (1997). Adsorptive stripping measurements. Anal. Chem. 69, 1657.

Wang, J., et. al. (1997). Renewable reagent electrochemical sensor for monitoring trace metals. Anal. Chem. 69, 2640.

Wang, J., et. al. (1997). Simultaneous adsorptive stripping voltammetric measurements of trace chromium, uranium, and iron. Electroanalysis. 9, 1247.

Wang, J., et. al. (2000). Lab-on-a-cable for monitoring priority contaminants. Anal. Chem. 71, 2659.

Wang, J., Grundler, P., Jasinski, M., & Tian, B. (1999). Hot-wire stripping potentiometric measurements of trace mercury. Anal. Chim. Acta. 396, 33.

Wang, J., Lou, D., & Horiuchi, T. (1998). Anodic stripping with collection at integrated carbon film microelectrode arrays. Electroanalysis. 10, 107.

Wang, J., Lu, J., Hocevar, S., Farias, P., & Ogorevc, B. (2000). Bismuth-coated carbon electrodes for anodic stripping voltammetry. 72, 3218.

Wang, J., Lu, J., Luo, D., & Tian, B. (1997). Simultaneous measurements of trace Cr and U using mixed ligand stripping analysis. Anal. Chim. Acta. 354, 275.

Wang, J., Lu, J., MacDonald, D., & Augelli, M. (1999). In-situ flow probe for improving the performance of electrochemical stripping analysis. Invited paper in Fres. Z. Anal. Chem. 364, 28.

Wang, J., Lu, J., Tian, B., MacDonald, D., & Olsen, K. (1999). Flow probe for in-situ electrochemical monitoring of trace chromium. Analyst. 124, 349.

Wang, J., Tian, B., & Lu, J. (1998). Electrochemical flow sensor for in-situ monitoring of total metal concentration. Anal. Communications. 35, 241.

Wang, J., Tian, B., Lu, J., & Luo, D. (1998). Renewable reagent enzyme inhibition biosensor for remote monitoring of cyanide. Electroanalysis. 10, 1034.

Wang, J., Tian, B., Lu, J., & MacDonald, D. (1998). Remote electrochemical sensor for monitoring trace mercury. Electroanalysis. 10, 399.

Wang, J., Tian, B., Lu, J., Olsen, K., & Yarnitsky, C. (1999). Stripping analysis into the 21st century: Faster, smaller, simpler, and better. Anal. Chim. Acta. 385, 429.

Publication Type: Patent

Wang, J. & Olsen, K. (1997) Remote Electrochemical Sensor. U.S. Patent No. 5,676, 820.

Wang, J. & Olsen, K. (1997). Remote electrochemical sensor. US5676820.

Wang, J. & Olsen, K. (1999). Renewable Electrochemical Sensors. U.S. Patent No. 5,942, 103.

Wang, J. & Olsen, K. (1999). Renewable electrochemical sensors. US5942103.

Project: 55108

Title: Monitoring Genetic & Metabolic Potential for In Situ Bioremediation: Mass Spectrometry

PI: Dr. Michelle V. Buchanan *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Costello, A. M. & Lidstrom, M. E. (1999, Nov.). Molecular characterization of functional and phylogenetic genes from natural populations of methanotrophs in lake sediments. Appl. Env. Microb. 65(11), 5066-5073.

Hurst, G. B., et. al. (1998). MALDI-TOF analysis of polymerase chain reaction products from methanotrophic bacteria. Analytical Chemistry. 70, 2693-2698.

Publication Type: Poster

Buchanan, M. V., et. al. (2000, Apr. 24-28). Monitoring genetic and metabolic potential for in situ bioremediation: Mass spectrometry. Poster presentation at the 2nd Annual Environmental Management Science Program Workshop, Atlanta, GA.

Hurst, G. B., et. al. (1998, Jan. 24-27). TOF-MS detection of PCR products. Poster presentation at the 10th Sanibel Conference on Mass Spectrometry. Sanibel Island, FL.

Hurst, G. B., Kim, Y., Weaver, K., & Buchanan, M. V. (1999, Jan. 12-16). PCR product size measurement using MALDI mass spectrometry. Poster presentation at the 7th DOE Human Genome Contractor-Grantee Workshop. Oakland, CA.

Hurst, G. B., Weaver, K., Buchanan, M. V., & Doktycz, M. J. (1997, Jun. 1-5). Analysis of PCR products using delayed-extraction MALDI-TOF. Proceedings of the 45th ASMS Conference on Mass Spectrometry and Allied Topics. Palm Springs, CA. 843.

Publication Type: Presentation

Buchanan, M. V., et. al. (1998, Jul. 27-30). Monitoring genetic and metabolic potential for in situ bioremediation: Mass spectrometry. Proceedings of the DOE Environmental Management Science Program Workshop. Chicago, IL. 252-253.

Hurst, G. B. (1999, Nov. 5-6). Characterization of bacteria using mass spectrometric detection of polymerase chain reaction products. Presentation at the 7th Symposium on Laser Spectoscopy at the Korea Atomic Energy Research Institute.

Hurst, G. B., et. al. (1999, Sep. 22). Monitoring genetic and metabolic potential for in situ bioremediation: Mass spectrometry. Presentation at the DOE-ORO EMSP Workshop, Oak Ridge, TN.

Kim, Y., Hurst, G. B., Doktycz, M. J., & Buchanan, M. V. (1999, Jun. 13-18). Improved spot homogeneity for DNA MALDI matrices. Proceedings of the 47th ASMS Conference on Mass Spectrometry and Allied Topics. Dallas TX.

Publication Type: Proceeding

Hurst, G. B., et. al. (1998, May 31 - Jun. 4). Identification of methanotrophic bacteria using the polymerase chain reaction with MALDI-TOF detection. Proceedings of the 46th ASMS Conference on Mass Spectrometry and Allied Topics. Orlando FL. 1202.

Hurst, G. B., Weaver, K., & Buchanan, M. V. (1997, Nov. 9-13). Improved mass spectrometric resolution for PCR product size measurement. Proceedings of the DOE Human Genome Program Contractor-Grantee Workshop VI, Santa Fe, NM. 39.

Weaver, K., Doktycz, M. J., Britt, P. F., Hurst, G. B., & Buchanan, M. V. (1998, May 31 - Jun. 4). 96-well microtiter-format purification of DNA for MALDI-TOF analysis. Proceedings of the 46th ASMS Conference on Mass Spectrometry and Allied Topics. Orlando FL. 1017.

Publication Type: Theses/Dissertations

Auman, A. (1999). Soluble methane monooxygenase-containing methanotrophs in lake Washington. Lidstrom, M. E. (Advisor). PhD dissertation at the Microbiology Department, University of Washington. Seattle, WA.

Costello, A. (1999, Apr.). Characterization of methanotrophic populations in lake Washington. Lidstrom, M. E. (Advisor). PhD dissertation at the California Institute of Technology, Environmental Engineering Science Department.

Project: 55328

Title: Novel Analytical Techniques Based on an Enhanced Electron Attachment Process

PI: Dr. Lal A. Pinnaduwage *Institution:* University of Tennessee at Knoxville

Publication Type: Journal

Ding, W., McCorkle, D. L., & Pinnaduwage, L. A. (1998). Enhanced negative ion formation by electron attachment to highly-excited molecules in a flowing plasma. J. Appl. Phys. 84, 3051.

Ding, W., Pinnaduwage, L. A., Tav, C., & McCorkle, D. L. (1999, Aug.). The role of high Rydberg states in enhanced O-formation in a pulsed O2 discharge. Plasma Sources Sci. T. 8(3), 384-391.

Mabel, A. M., Lin, S. H., & Pinnaduwage, L. A. (1998). Potential energy surfaces of H2. Chem. Phys. Lett. 285, 114.

Nagesha, K. & Pinnaduwage, L. A. (1998). O-formation from O2 via Rydberg-Rydberg electron transfer. J. Chem. Phys. 109, 7124.

Nagesha, K. & Pinnaduwage, L. A. (1999, Oct. 15). Magnetic and electric field induced enhancements in laser-induced anion formation. Chem. Phys. Lett. 312(1), 19-27.

Pinnaduwage, L. A. & Zhu, Y. (1997). Long-time stability of superexcited high-Rydberg molecular states. Chem. Phys. Lett. 277, 147.

Pinnaduwage, L. A. & Zhu, Y. (1998). High-Rydberg fragment formation via core dissociation of superexcited Rydberg molecules. J. Chem. Phys. 108, 6633.

Pinnaduwage, L. A., et. al. (1999). Enhanced electron attachment to Rydberg states in molecular hydrogen volume discharges. J. Appl. Phys. 85, 7064.

Pinnaduwage, L. A., McCorkle, D. L., & Ding, W. (1997, Dec. 22). Enhanced electron attachment to highly excited molecules using a plasma mixing scheme. Appl. Phys. Lett. 71(25), 3634-3636.

Pinnaduwage, L. A., Nagesha, K., Zhu, Y., Buchanan, M. V., & Hurst, G. B. (1999, Oct. 28). Laser-enhanced negative ion mass spectroscopy for weakly electron-attaching species. Int. J. Mass. Spectrom. 193(1), 77-86.

Tav, C. & Pinnaduwage, L. A. (2000, in press). Enhanced dissociative electron attachment to laser-excited benzene. Journal of Applied Physics.

Publication Type: Presentation

Ding, W. X., Pinnaduwage, L. A., Tav, C., & McCorkle, D. L. (1999, Mar. 20-26). O formation by electron attachment to high Rydberg states. Presentation at the 1999 Centennial Meeting of the American Physical Society. Atlanta, GA.

Nagesha, K. & Pinnaduwage, L. A. (1999, Oct. 5-8). Magnetic and electric field induced enhancements in laser induced anion formation. 52nd Annual Gaseous Electronics Conference. Norfolk, Virginia.
Pinnaduwage, L. A. (1997, Jun. 29-Jul. 7). Implications of electron attachment to highly-excited states in pulsed power discharges. 11th IEEE Pulsed Power Conference. Baltimore, MD.

Pinnaduwage, L. A. (2000, Jun. 19-21). Novel analytical techniques based on an enhanced electron attachment process. Presentation at the Environmental Management Science Program Sensors Initiative Workshop, Idaho Falls, ID.

Pinnaduwage, L. A. (2000, Oct. 24-27). Electron attachment to Rydberg states and its implications for low-temperature plasmas. Invited presentation at the 53rd Annual Gaseous Electronics Conference, Houston, TX.

Pinnaduwage, L. A., Buchanan, M. V., & Hurst, G. B. (1998, Jul. 27-30). Novel analytical techniques based on an enhanced electron atachment process. Presented at the Environmental Management Science Program Workshop. Chicago, IL.

Pinnaduwage, L. A., Buchanan, M. V., & Hurst, G. B. (2000, Apr. 24-28). Novel analytical techniques based on an enhanced electron attachment process. Presentation at the Environmental Management Science Program Workshop, Atlanta, GA.

Pinnaduwage, L. A., Ding, W. & McCorkle, D. L. (1999, Oct. 5-8). Negative ion formation in pulsed plasmas. 52nd Annual Gaseous Electronics Conference. Norfolk, VA.

Pinnaduwage, L. A., Ding, W. X., & McCorkle, D. L. (1999, Mar. 20-26). Enhanced electron attachment to Rydberg states in molecular hydrogen volume discharges. Presentation at the 1999 Centennial Meeting of the American Physical Society. Atlanta, GA.

Pinnaduwage, L. A., Ding, W. X., & McCorkle, D. L. (1998, Jun. 27 - Jul. 3). Enhanced electron attachment to superexcited Rydberg states of molecular hydrogen using a plasma mixing scheme. Pavlo, P. (Ed.)., Proceedings of the 1998 International Congress on Plasma Physics. Prague, Czech Republic. 129-132.

Pinnaduwage, L. A., Ding, W. X., McCorkle, D. L., & Ma, C. Y. (1999, Jun. 27-30). Implications of electron attachment to highly-excited states of molecules and its applications in pulsed plasmas. 12th IEEE Pulsed Power Conference. Monterey, CA.

Tav, C. & Pinnaduwage, L. A. (1999, Oct. 5-8). Dissociative electron attachment to laser-excited benzene. 52nd Annual Gaseous Electronics Conference. Norfolk, VA.

Zhu, Y. & Pinnaduwage, L. A. (1997, Oct. 6-9). Long-time stability of superexcited high Rydberg molecular states. 50th Annual Gaseous Electronics Conference. Madison, WI.

Publication Type: Proceeding

Pinnaduwage, L. A, Ding, W. X., & McCorkle, D. L. (1999). Enhanced electron attachment to superexcited Rydberg states of molecular hydrogen using a plasma mixing scheme. Pavlo, P. (Ed). Proceedings of the 1998 International Congress on Plasma Physics. Prague, Czech Republic. 129-132.

Pinnaduwage, L. A. (1997, Jun. 29 - Jul. 2). Implications of electron attachment to highly-excited states in pulsed power discharges. Cooperstein, G. & Vitkovitsky, I. (Eds.). Digest of Technical Papers of the 11th IEEE Pulsed Power Conference held in Baltimore, MD. IEEE Publishing Services, New York, NY. 1048-1053.

Pinnaduwage, L. A., Ding, W. X., McCorkle, D. L., & Ma, C. Y. (1999). Enhanced electron attachment to highly-excited molecules and its applications in pulsed plasmas. Digest of Technical Papers of the 12th IEEE Pulsed Power Conference, IEEE Publishing Services, New York, NY. 1322-1325.

Publication Type: Theses/Dissertations

Tav, C. (2000, Aug.). Enhanced electron attachment to vibrationally and electronically excited molecules. PhD dissertation.

Project: 70010 (Renewal of Project No. 54674)

Title: Spectroelectrochemical Sensor for Technetium Applicable to the Vadose Zone
PI: Dr. William R. Heineman *Institution:* University of Cincinnati

Publication Type: Presentation

Bryan, S. A., et. al. (2000, Aug.). Selective ion-exchange films for technetium sensors. 220th American Chemical Society National Meeting. Washington, D. C.

Conklin, S., Heineman, W. R., & Seliskar, C. J. (2000, May 16-19). Evaluation of silica composites containing quarternized poly(4-vinylpyridine) as an anion exchanger of pertechnetate, TcO4 ions for use in chemical sensors. 32nd American Chemical Society Central Regional Meeting (CMACS). Covington, KY.

Heineman, W. R. (2000, Apr. 29). Strategies for new chemical sensors. Sensor Technology for the New Millenium Symposium. University of Pittsburgh. Pittsburgh, PA.

Heineman, W. R. (2000, Jun. 4-9). Strategies for new chemical sensors. 3rd Mediterranean Basin Conference on Analytical Chemistry (MBCAC III). Antalya, Turkey.

Heineman, W. R. (2000, Sept. 19-20). Chemical sensors for monitoring during stewardship. Post Closure Stewardship Technology Needs Meeting. University of Cincinnati. Cincinnati, OH.

Heineman, W. R., et. al. (2000, Jun. 11-15). Combining electrochemistry and spectroscopy into a single sensor. 8th International Conference on ElectroAnalysis (ESEAC/SEAC 2000). Bonn, Germany.

Heineman, W. R., Seliskar, C. J., Bryan, S. A., & Hubler, T. L. (2000, Apr. 24-27). Spectoelectrochemical sensor for Ferrocyanide and Technetium. Environmental Management Science Program National Workshop. Atlanta, GA.

Maizels, M., et. al. (2000). Novel spectroelectrochemical sensor for ferrocyanide in Hanford waste simulant. In Eller, P. G. & Heineman, W. R. (Eds.). Nuclear Site Remediation: First Accomplishments of the Environmental Management Science Program. American Chemical Society Symposium Series. 778. Washington, D. C.

Rarog, T., Seliskar, C. J., & Heineman, W. R. (2000, May 16-19). Cu2+ bait and switch sensor. 32nd American Chemical Society Central Regional Meeting (CMACS). Covington, KY.

Zudans, I., Seliskar, C. J., & Heineman, W. R. (2000, May 16-19). Optical study of thin sol-gel films on ITO for spectroelectrochemical sensor. 32nd American Chemical Society Central Regional Meeting (CMACS). Covington, KY.

Publication Type: Theses/Dissertations

Maizels, M. (2000). Spectroelectrochemical sensor for technetium applicable to the vadose zone. PhD. Dissertation. University of Cincinnati. Cincinnati, OH.

Ross, S. (2000). Spectroelectrochemical sensor for technetium applicable to the vadose zone. PhD. Dissertation. University of Cincinnati. Cincinnati, OH.

Wanamaker, M. (2000). Spectroelectrochemical sensor for technetium applicable to the vadose zone. Masters Thesis. University of Cincinnati. Cincinnati, OH.

Project: 70179

Title: Radionuclide Sensors for Water Monitoring

PI: Dr. Jay W. Grate *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

DeVol, T. A., Duffey, J. M., & Paulenova, A. (2001, in press). Combined extraction chromatography and scintillation detection for on-line and off-line monitoring of strontium in aqueous solutions. J. Radioanalytical and Nuclear Chemistry. 249(2).

DeVol, T. A., Egorov, O. B., Roane, J. B., Paulenova, A., & Grate, J. W. (2001, in press). Extractive scintillating microspheres for 99Tc quantification in aqueous solutions. J. Radioanalytical and Nuclear Chemistry. 249(1).

DeVol, T. A., Roane, J. E., Williamson, J. M., Duffey, J. M., & Harvey, J. T. (2000). Development of scintillating extraction media for separation and measurement of charged-particle emitting radionuclides in aqueous solutions. Radioactivity and Radiochemistry, 11(1), 34-46.

Tan, H., Fjeld, R. A., & DeVol, T. A. (2000, in press). Digital alpha/beta pulse shape discrimination of CsI: Tl for on-line measurement of aqueous radioactivity. IEEE Trans. Nucl. Sci.

Publication Type: Presentation

DeVol, T. A. (2000, May 16). Chromatographic separation and measurement of charged-particle emitting radionuclides. Invited speaker at Eichrom Technologies, Inc. Eastern Users' Group Workshop, Augusta, GA.

DeVol, T. A., Duffey, J. M., & Paulenova, A. (2000, Sep. 24-28). Combination extraction chromatography and scintillation detection resin for quantification of strontium in aqueous solutions. Spectrum 2000, Chattanooga, TN.

DeVol, T. A., Duffey, J. M., & Paulenova, A. (2000, Apr. 9-14). Combined extraction chromatography and scintillation detection for on-line and off-line monitoring of strontium in aqueous solutions. Fifth International Conference on Methods and Applications of Radioanalytical Chemistry (MARC V), Kailua-Kona, HI.

DeVol, T. A., Egorov, O. B., Roane, J. E., Paulenova, A., & Grate, J. W. (2000, Jul. 16-21). Extractive scintillating microspheres for 89,90Sr quantification in aqueous solutions. Gordon Conference on Nuclear Waste and Energy, New London, NH.

DeVol, T. A., Egorov, O. B., Roane, J. E., Paulenova, A., & Grate, J. W. (2000, Apr. 9-14). Extractive scintillating microspheres for 99Tc quantification in aqueous solutions. Fifth International Conference on Methods and Applications of Radioanalytical Chemistry (MARC V), Kailua-Kona, HI.

Egorov, O. B. & Grate, J. W. (2000, Nov. 12-17). Automated radionuclide separations, analysis, and sensing. Invited presentation at the 46th Annual Conference on Bioassay, Analytical, and Environmental Radiochemistry. Seattle, WA.

Tan, H. & DeVol, T. A. (2000, Jun. 24-29). Development of a digital alpha/beta pulse shape discriminating system utilizing CsI(Tl)/photodiode. 44th Annual Meeting of the Health Physics Society, Denver, CO.

Project: 73808 (Renewal of Project No. 60197)

Title: Microsensors for In-Situ Chemical, Physical, & Radiological Characterization Mixed Waste

PI: Dr. Thomas G. Thundat *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

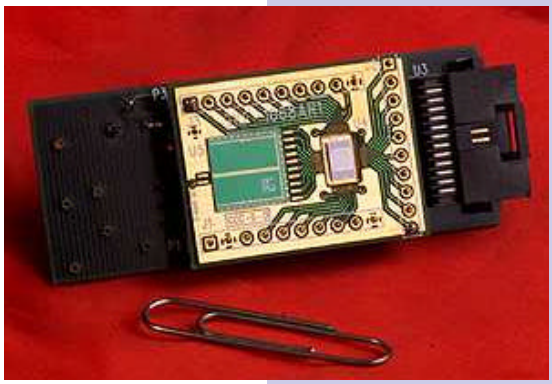
Ji, H. - F., et. al. (2000). A novel self-assembled monolayer (SAM) coated microcantilver for low level caesium detection. Chem. Commun. 6, 457-458.

Thundat, T. G. & Maya, L. (1999). Monitoring chemical and physical changes on sub-nanogram quantities of platinum oxide. Surf. Sci. Lett. 430, L546.

Publication Type: Patent

Ji, H.- F., Thundat, T. G., Brown, G. M., Britt, P. F., & Dabestani, R. (2000). Microcantilever ion sensors. (invention disclosure submitted).

Thundat, T. G. & Doktycz, M. J. (2000). Micromechanical scanning differential calorimeter. ESID-1777-X (all claims allowed).



The photograph is a working device of a microcantilever array with 10 individual cantilever elements. All the signal processing electronics is right on the chip. With a battery this device will be able to sense 10 different analytes simultaneously. [see Project #73808, renewal of #60197]

Thundat, T. G. & Wachter, E. A. (2000). Tunable frequency cantilevers. ESID-1739-X (patent pending).

Thundat, T. G. (2000). Micro-mechanical potentiometric sensors. U. S. Patent # 6,016,689.

Thundat, T. G. (2000). Micro-mechanical potentiometric sensors. ERID-0235, (all claims allowed).

Thundat, T. G. (2000). Microcantilever detector for landmines, unexploded ordances, and explosives. U. S. Patent # 5,918,263.

Thundat, T. G. (2000). Uncoated microcantilevers as chemical sensors. ERID-0545 (all claims allowed).

Thundat, T. G., Datskos, P. G., & Oden, P. I. (2000). Noncontact infrared thermometer and IR detection without emissivity correction. U. S. Patent # 6,050,722.

Thundat, T. G., Oden, P. I., & Datskos, P. G. (2000). Wavelength dispersive infrared detector and spectrometer using microcantilevers. (patent pending).

Thundat, T. G., Oden, P. I., Warmack, R. J., & Finot, E. L. (2000). Micromechanical transient sensor for measuring viscosity and specific gravity. ERID-0516 (patent pending).

Thundat, T. G., Warmack, R. J., & Wachter, E. A. (2000). Electromagnetic and nuclear radiation detector using micromechanical sensors. ESID-1604 (all claims allowed).

Publication Type: Presentation

Thundat, T. G. (1997). Microcantilever array sensors. Materials Science Dept. Colloquium, University of Illinois - Urbana, Urbana, IL.

Thundat, T. G. (1997). Microcantilever sensors. 37th ORNL-DOE Conference on Analytical Chemistry in Energy Technology, Gatlinburg, TN.

Thundat, T. G. (1997). Micromechanical array sensors. Alabama Materials Research Society Meeting, Huntsville, AL.

Thundat, T. G. (1998). Imaging and non-imaging applications of scanning probe microscopy. UT Materials Science Dept., Knoxville, TN.

Thundat, T. G. (1998). Micromechanical array sensors for chemical and biological detection. University of Bourgogne, Laboratoire de Photoelectricite, Dijon, France.

Thundat, T. G. (1999). Chemical, physical, biological detection using microcantilevers. Columbus Section American Chemical Society Meeting, Columbus, OH.

Thundat, T. G. (1999). Microcantilever chemical sensors. Micro Nano Technology Conference, Pasadena, CA.

Thundat, T. G. (1999). Microcantilever sensors. Materials Sciences Dept., Ohio State University, Columbus, OH.

Thundat, T. G. (1999). Micromechanical chemical and biological sensors. University of California, Berkeley, CA.

Thundat, T. G. (2000). Microcantilever sensors. 2nd Annual Environmental Management Science Program National Workshop, Atlanta, GA.

Thundat, T. G. (2000). Microcantilever sensors. DOE BES Workshop on Nanotechnology, University of California, Berkeley, CA.

Thundat, T. G. (2000). Microsensors for in-situ chemical, physical, and radiological characterization of mixed waste. 2nd Annual Environmental Management Science Program National Workshop, Atlanta, GA.

Thundat, T. G., Hu, Z., Chen, G. Y., & Warmack, R. J. (1999). Elastic effects of coating films on resonance response of microcantilevers. 1999 APS March Meeting, Atlanta, GA.

Thundat, T. G., Oden, P. I., & Warmack, R. J. (1998). Microcantilever array sensors. WATTEC-98, Knoxville, TN.

Thundat, T. G., Oden, P. I., Doktycz, M. J., & Warmack, R. J. (1998). Micromechanical sensors. Gordon Research Conference, New England College, Henniker, NH.

Thundat, T. G., Oden, P. I., Warmack, R. J., & Brown, G. M. (1998). Microcantilever sensors for environmental monitoring. Electrochemical Society Meeting, San Diego, CA.

Publication Type: Proceeding

Hu, Z., Thundat, T. G., & Warmack, R. J. (2000). Metal coated microcantilever hydrogen and mercury sensors. Butler, M., Yamazoe, N., Vanysek, P., & Aizawa, M. (Eds). Chemical Sensors IV, ECS Proceedings 99-23, 347-354.

Thundat, T. G., et. al. (2000). Highly selective microcantilever sensor for Cs ion detection. Butler, M., Yamazoe, N., Vanysek, P., & Aizawa, M. (Eds.). Chemical Sensors IV, ECS Proceedings 99-23, 314-319.

Publication Type: Theses/Dissertations

Hu, Z. (2000, May). Chemo-electro-mechanical properties by microcantilever sensors. Ph. D. dissertation.

Biogeochemistry

Project: 54790

Title: Microbial Mineral Transformations at the Fe(II)/Fe(III) Redox Boundary for Solid Phase Capture of Strontium and Other Metal/Radionuclide Contaminants

PI: Dr. F. Grant Ferris *Institution:* University of Toronto

Publication Type: Journal

Howell, J. R., Donahoe, R. J., Roden, E. E., & Ferris, F. G. (1998). Effects of microbial iron oxide reduction on pH and alkalinity in anaerobic bicarbonate-buffered media: Implications for metal mobility. Mineralogical Magazine 62A, 657-658.

Howell, J. R., Donahoe, R. J., Roden, E. E., & Ferris, F. G. (1998). Effects of microbial iron oxide reduction on pH and alkalinity in anaerobic bicarbonate-buffered media: Implications for metal mobility. Mineralogical Magazine. 62A, 657-658.

Leonardo, M. R., Keith, V. K., Ferris, F. G., & Roden, E. E. (1999, Aug. 22). Immobiliztion of strontium during carbonate mineral formation coupled to microbial reduction of amorphous Fe(III) oxide. Abstr. Pap. Am. Chem. S. 218, U1044-U1044, Part 1.

Small, T. S., Warren, L. A., Roden, E. E., & Ferris, F. G. (1999, Dec. 15). Sorption of strontium by bacteria, Fe(III) oxide, and bacteria-Fe(III) oxide composites. Environmental Science and Technology, 33(24), 4465-4470.

Publication Type: Presentation

Howell, J. R., Donahoe, R. J., & Roden, E. E. (1997). Effects of micobial iron oxide reduction on pH and alkalinity in anaerobic bicarbonate-buffered media. American Geophysical Union Fall Meeting.

Keith, V. K. & Roden, E. E. (1999). Immobilization of aqueous strontium during bacterial reduction of synthetic Fe(III) oxides. American Society for Microbiology Annual Meeting.

Leonardo, M. R., Ferris, F. G., & Roden, E. E. (1999). Sr2+ immobilization by authigenic carbonate precipitation under iron-reducing conditions. American Society for Microbiology Annual Meeting.

Leonardo, M. R., Ferris, F. G., & Roden, E. E. (1998). Analysis of iron-carbonate mineral formation during microbial reduction of synthetic amorphous iron oxide. American Society for Microbiology General Meeting.

Maurice, P. A., Warren, L. A., Ferris, F. G. (1998). Calcite precipitation by B. pasteurei: AFM imaging of microbial-mineral interactions. Geological Society of America Annual Meeting.

Maurice, P.A., Warren, L. A., & Ferris, F. G. (1998). Calcite precipitation by B. pasteurei: AFM imaging of microbial-mineral interactions. Geological Society of America Annual Meeting. Toronto, Canada.

Parmar, N., Warren, L. A. & Ferris, F. G. (1998). Solid phase capture of strontium by the iron reducing bacteria Shewenella alga. Geological Society of America Annual Meeting. Toronto, Canada.

Parmar, N., Warren, L. A., & Ferris, F. G. (1999). Impact of Fe(III) reduction on Fe(II)/Fe(III) mineral transformation and solid phase capture of strontium. XIV International Symposium on Environmental Biogeochemistry.

Roden, E. E., Leonardo, M. R., & Ferris, F. G. (1999). Immobilization of strontium during carbonate mineral-formation coupled to microbial Fe(III) oxide reduction. XIV International Symposium on Environmental Biogeochemistry.

Roden, E. E., Leonardo, M. R., Keith, V. K., & Ferris, F. G. (1999). Immobilization of aqueous strontium during carbonate mineral formation coupled to microbial Fe(III) oxide reduction. International Symposium on Subsurface Microbiology.

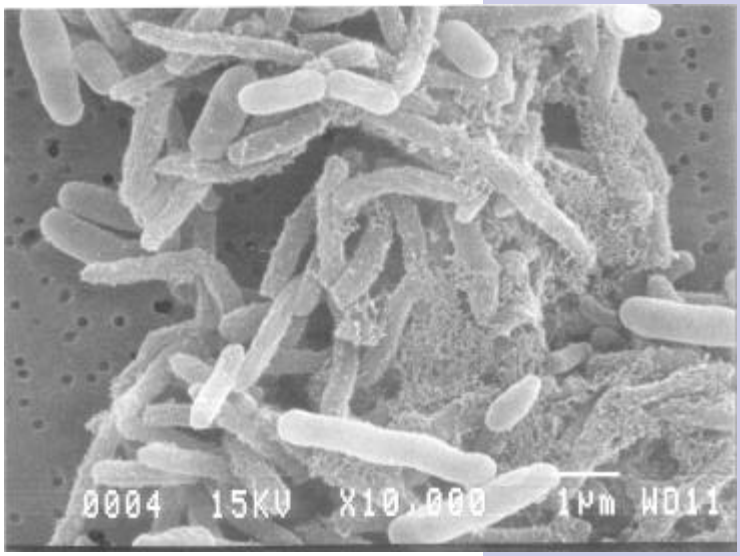
Small, T. D., Warren, L. A., & Ferris, F. G. (1998). Strontium sorption to bacterial and Fe oxide surfaces. Geological Society of America Annual Meeting.

Small, T. D., Warren, L. A., Roden, E. E., & Ferris, F. G. (1999). Sorption of strontium by bacteria, Fe(III) oxide and bacterial-Fe(III) oxide composites. XIV International Symposium on Environmental Biogeochemistry.

Small, T.D., Warren, L. A., & Ferris, F. G. (1998). Strontium sorption to bacterial and Fe oxide surfaces. Geological Society of America Annual Meeting. Toronto, Canada.

Warren, L. A., Ferris, F. G., & Roden, E. E. (1997). Strontium reactions at Shewenella and hydrous ferric oxide (HFO) surfaces. Geological Society of America Annual Meeting.

Warren, L. A., Parmar, N., & Ferris, F. G. (1998). Strontium, uranyl, and copper incorporation in bacterially mediated calcite precipitation. Geological Society of America Annual Meeting. Toronto, Canada.



A scanning electron microscope image showing dissimilatory iron-reducing bacteria with adherent hydrous ferric oxide. [see Project #54790]

Publication Type: Proceeding

Warren, L. A. & Ferris, F. G. (1998). Solid phase partitioning of uranium and copper in the presence of hydrous ferric oxide and bacteria. Arehart, G. B. & Hulston, J. R. (Eds.) Proceedings of the 9th International Symposium on Water-Rock Interactions. Balkema, Rotterdam. 115-117.

Publication Type: Theses/Dissertations

Howell, J. R. (1998). Effects of microbial Fe(III) oxide reduction on pH, DIC, and carbonate mineral formation: Implications for metal mobility. M. S. Thesis. Department of Geology, University of Alabama, Tuscaloosa, Alabama.

Keith, V. K. (2000). Immobilization of aqueous strontium during bacterial reduction of synthetic goethite. M. S. Thesis. Department of Biological Sciences, University of Alabama, Tuscaloosa, Alabama.

Small, T. D. (2000). Sorption of strontium to bacteria, Fe(III) oxide, and bacteria-Fe(III) oxide composites in relation to contaminant fate. M. S. Thesis, Department of Geology, University of Toronto, Toronto, Ontario, Canada.

Project: 55164

Title: Advanced Experimental Analysis of Controls on Microbial Fe(III) Oxide Reduction

PI: Dr. Eric E. Roden *Institution:* University of Alabama

Publication Type: Journal

Roden, E. E. & Urrutia, M. M. (1999). Ferrous iron removal stimulates microbial iron(III) oxide reduction in semicontinuous cultures. Environ. Sci. Technol. 33, 1847-1853.

Roden, E. E., Urrutia, M. M., & Mann, C. J. (2000). Bacterial reductive dissolution of crystalline Fe(III) oxide in continuous-flow column reactors. Appl. Environ. Microbiol. 66, 1062-1065.

Sobolev, D. & Roden, E. E. (2001). Suboxic deposition of ferric iron by bacteria in opposing gradients of Fe(II) and oxygen at circumneutral pH. Appl. Environ. Microbiol. 67, 1328-1334.

Urrutia, M. M., Roden, E. E., & Zachara, J. M. (1999). Influence of aqueous and solid-phase Fe(II) complexants on microbial reduction of crystalline Fe(III) oxides. Environ. Sci. Technol. 33, 4022-4028.

Urrutia, M. M., Roden, E. E., Fredrickson, J. K., & Zachara, J. M. (1998). Microbial and surface chemistry controls on reduction of synthetic Fe(III) oxide minerals by the dissimilatory iron-reducing bacterium Shewanella alga. Geomicrobiol. J. 15, 269-291.

Project: 55388

Title: Stable Isotopic Investigations of In Situ Bioremediation of Chlorinated Organic Solvents

PI: Dr. Neil C. Sturchio *Institution:* Argonne National Laboratory

Publication Type: Journal

Dayan, H., Abrajano, T., Sturchio, N. C., & Winsor, L. (1999). Carbon isotopic fractionation during reductive dechlorination of chlorinated solvents by metallic iron. Organic Geochemistry. 30, 755-763.

Heraty, L. J., Fuller, M. E., Huang, L., Abrajano, T., & Sturchio, N. C. (1999). Carbon and chlorine isotopic fractionation during microbial degradation of dichloromethane. Organic Geochemistry. 30, 793-799.

Holt, B. D., Sturchio, N. C., Abrajano, T. A., & Heraty, L. J. (1997). Conversion of chlorinated organic compounds to carbon dioxide and methyl chloride for isotopic analysis of carbon and chlorine. Analytical Chemistry. 69, 2727-2733.

Huang, L., Sturchio, N. C., Abrajano, T., Heraty, L. J., & Holt, B. D. (1999). Carbon and chlorine isotope fractionation of chlorinated aliphatic hydrocarbons by evaporation. Organic Geochemistry. 30, 777-785.

Reddy, C. M., et. al. (1999, in press). Stable chlorine isotopes in semivolatile organic compounds. Environmental Science and Technology.

Sturchio, N. C., et. al. (1998). Stable chlorine isotope investigation of natural attenuation of trichloroethene in an aerobic aquifer. Environmental Science and Technology. 32, 3037-3042.

Publication Type: Patent

Holt, B. D. & Sturchio, N. C. (1999, Aug. 28). Method for isotopic analysis of chlorinated organic compounds. U. S. Patent # 5,942,439.

Holt, B. D. & Sturchio, N. C. Method for isotopic analysis of chlorinated organic compounds. US #5,942,439.

Publication Type: Presentation

Dayan, H., Abrajano, T., Heraty, L., Huang, L., & Sturchio, N. C. (1997). Isotopic fractionation during reductive dehalogenation of chlorinated ethenes by metallic iron. Geological Society of America Abstracts with Programs. 29(6), A185.

Heraty, L. J., et. al. (1999, Oct. 25-28). Microbial degradation of chlorinated aliphatic hydrocarbons: Field investigations using stable carbon and chlorine isotopes. Geological Society of America 1999 Annual Meeting. Denver, CO.

Holt, B. D. & Sturchio, N. C. (1996). High temperature method for conversion of chlorinated organic compounds to CH3Cl and CO2 for isotopic analysis of chlorine and carbon. Abstracts of Papers of the American Chemical Society. 212, 154-ENVR.

Holt, B. D., Heraty, L. J., & Sturchio, N. C. (1999, Aug. 22-26). Extraction of chlorinated aliphatic hydrocarbons from water for isotopic analysis of chlorine and carbon. American Chemical Society 218th National Meeting. New Orleans, LA.

Huang, L., Sturchio, N. C., Heraty, L., & Abrajano, T. (1998, Aug.). Chlorine and carbon isotopic fractionations of aliphatic hydrocarbons in evaporation processes: Implications for biodegradation. 9th International Conference on Geochronology, Cosmochronology, and Isotope Geology. Beijing, China.

Reddy, C. M., et. al. (1999, Aug. 22-27). Chlorine isotope ratios of semi-volatile chlorinated organic compounds. Ninth Annual V. M. Goldschmidt Conference. Cambridge, MA.

Sturchio, N. C., Abrajano, T., Heraty, L., Huang, L., & Clausen, J. (1997). Stable isotope investigation of natural attenuation of trichloroethene at the Paducah Gaseous Diffusion Plant. Geological Society of America Abstracts with Programs. 29(6), A185.

Sturchio, N. C., et. al. (1997, Sept. 22-26). Carbon and chlorine isotopic studies of biodegradation of chlorinated volatile organics. 18th International Meeting on Organic Geochemistry, Maastricht, The Netherlands.

Sturchio, N. C., et. al. (2000, May 22-25). Stable isotope ratios of chlorinated aliphatic hydrocarbons in contaminated aquifers. Second International Conference on Remediation of Chlorinated and Recalcitrant Compounds. Monterey, CA.

Sturchio, N. C., Heraty, L. J., Holt, B. D., Huang, L., & Abrajano, T. (1999, Aug. 22-27). Stable isotope investigations of the chlorinated aliphatic hydrocarbons. Ninth Annual V. M. Goldschmidt Conference. Cambridge, MA.

Sturchio, N. C., Heraty, L. J., Holt, B. D., Huang, L., & Abrajano, T. (1999, Jun. 7-9). Stable isotope investigations of chlorinated aliphatic hydrocarbons. Proceedings of the Second International Symposium on Integrated Technical Approaches to Site Characterization. Argonne, IL. 151-156.

Publication Type: Proceeding

Sturchio, N. C., Heraty, L., Holt, B., Huang, L., & Abrajano, T. (1999). Stable isotope investigations of chlorinated aliphatic hydrocarbons. Proceedings of the Second International Symposium on Integrated Technical Approaches to Site Characterization. Argonne, IL. 151-156.

Project: 70063 (Renewal of Project No. 54666)

Title: Biodegradation of Chlorinated Solvents: Reactions Near DNAPL and Enzyme Function

PI: Dr. Perry L. McCarty *Institution:* Stanford University

Publication Type: Journal

Haston, Z. C. & McCarty, P. L. (1999). Chlorinated ethene half-velocity coefficients (K S) for reductive dehalogenation. Environmental Science and Technology. 33(2), 223-226.

Rosner, B., McCarty, P. L., & Spormann, A. M. (1997). In vitro studies on reductive vinyl chloride dehalogenation by an anaerobic mixed culture. Appl. Environ. Microbiol. 63(11), 4139-4144.

Yang, Y. & McCarty, P. L. (1998). Competition for hydrogen within a chlorinated solvent dehalogenating mixed culture. Environmental Science and Technology. 32(22), 3591-3597.

Yang, Y. & McCarty, P. L. (1999). Response to "Comment on competition for hydrogen within a chlorinated solvent dehalogenating anaerobic mixed culture." Environmental Science & Technology. 33(12), 2128.

Yang, Y. & McCarty, P. L. (2000, in press). Biomass, oleate, and other possible substrates for chloroethene reductive dehalogenation. Bioremediation Journal.

Yang, Y. R. & McCarty, P. L. (2000, Jul. 15). Biologically enhanced dissolution of tetrachloroethene DNAPL. Environ. Sci. Technol. 34(14), 2979-2984.

Publication Type: Theses/Dissertations

Haston, Z. C. (1999). Factors affecting growth and utilization in the anaerobic dehalogenation of chlorinated ethenes. Ph.D. Dissertation. Stanford University. Stanford, CA.

Project: 70165

Title: Integrated Field, Laboratory, and Modeling Studies to Determine the Effects of Linked Microbial and Physical Spatial Heterogeneity on Engineered Vadose Zone Bioremediation

PI: Dr. Fred J. Brockman *Institution:* Pacific Northwest National Laboratory

Publication Type: Presentation

Bradley, S. N., Spadoni, T. S., & Brockman, F. J. (2001, May 20-24). Colonization behavior of Pseudomonas stutzeri KC in static unsaturated porous media columns. American Society for Microbiology General Meeting. Orlando, FL.

Project: 73784 (Renewal of Project No. 55267)

Title: Microbially Mediated Immobilization of Contaminants Through In Situ Biostimulation: Scale up of EMSP project 55267

PI: Dr. Philip M. Jardine *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Barnett, M. O., Jardine, P. M., Brooks, S. C., & Selim, H. M. (2000). Adsorption and transport of U(VI) in subsurface media. Soil Sci. Soc. Am. J. 64, 908-917.

Brooks, S. C. & Barnett, M. O. (1999, in press). Uranium sorption to bacterial cells as a related to metal reduction capabilities in the presence of porous media. Appl. and Eniron. Micro.

Brooks, S. C., Carroll, S. L., & Jardine, P. M. (1999). Sustained bacterial reduction of Co(III)EDTA in the presence of competing geochemical oxidation during dynamic flow. Environ. Sci. Technol. 33, 3002-3011.

Fendorf, S. E., Jardine, P. M., Patterson, R. R., Taylor, D. L., & Brooks, S. C. (1999, Oct.). Pyrolusite surface transformations measured in real-time during the reactive transport of Co(II)EDTA(2-). Geochim. Cosmochim. Acta. 63(19-20), 3049-3057.

Jardine, P. M., et. al. (1999). Fate and transport of hexavalent chromium in undisturbed heterogeneous soil. Environ. Sci. Technol. 33, 2939-2944.

Jardine, P. M., et. al. (1999). Quantifying diffusive mass transfer in fractured shale bedrock. Water Resour. Res. 35, 2015-2030.

Saiers, J. E., Guha, H., Jardine, P. M., & Brooks, S. C. (2000, in press). Development and evaluation of a mathematical model for the transport and oxidation-reduction of CoEDTA. Water Resourc. Res.

Publication Type: Other

Jardine, P. M., Brooks, S. C., Wilson, G. V., & Sanford, W. E. (2000, in press). Basic research strategies for resolving remediation needs in contaminated fractured subsurface media. Faybishenko, B. (Ed.), Dynamics of Fluids in Fractured Rocks: Concepts and Recent Advances. American Geophysical Union, Geophysical Monograph Series.

Jardine, P. M., O'Brien, R., Wilson, G. V., & Gwo, J. P. (1998). Experimental techniques for confirming and quantifying physical nonequilibrium processes in soils. Selim, H. M. & Ma, L. (Eds.), Physical Nonequilibrium in Soils: Modeling and Application. Ann Arbor Press, Inc. Chelsea, MI. 243-271.

Jardine, P. M., Wilson, G. V., Luxmoore, R. J., & Gwo, J. P. (2000, in press). Conceptual model of vadose-zone transport in fractured weathered shales. Hsieh, P. A. (Ed.), Conceptual Models of Flow and Transport in the Fractured Vadose Zone. National Research Council.

Publication Type: Presentation

Bostick, B. C., Fendorf, S. E., Barnett, M. O., Jardine, P. M., & Brooks, S. C. (2000, Nov. 5-9). Uranyl surface species formed during reactive transport through subsurface media. Soil Science Society of America, Minneapolis, MN.

Brooks, S. C., & Jardine, P. M. (1997, Oct. 26-31). Bacterial reduction of toxic metals during dynamic flow. American Society of Agronomy. Anaheim, CA.

Fendorf, S., Jardine, P. M., & Brooks, S. C. (1997, Apr. 13-17). Sorption induced inhibition of redox reaction involving manganese oxides. American Chemical Society. San Francisco, CA.

Guha, H., Saiers, J. E., Jardine, P. M., & Brooks, S. C. (1998, Dec. 6-10). Development and evaluation of a mathematical model for oxidation, sorption, and transport of Co(II)EDTA 2-. American Geophysical Union. San Francisco, CA.

Jardine, P. M. (1997, Oct. 12). Geochemical processes governing the fate and transport of Cr(III) and Cr(VI) in soils. Soil Science Society of America. Anaheim, CA.

Jardine, P. M. (1997, Oct. 26). Bacterial reduction of toxic metals during dynamic flow. Science Society of America. Anaheim, CA.

Jardine, P. M., et. al. (1999, Feb. 6-10). Basic research strategies for resolving remediation needs in contaminated fractured subsurface media. Symposium on Dynamics of Fluids in Fractured Rocks: Concepts and Recent Advances. Lawrence Berkeley National Laboratory. Berkeley, CA.

Jardine, P. M., Wilson, G. V., Sanford, W. E., & Luxmoore, R. J. (1998, May 14-16). Exploring subsurface transport mechanisms in fractured media at laboratory and field scales. Conference on “Mass transport in fractured aquifers and aquitards” Geological Institute, Unversity of Copenhagen, Denmark.

Mayes, M. A., Reedy, O. C., Larsen, I. L., Brooks, S. C., & Jardine, P. M. (1997,Oct. 26-31). Multispecies contaminant transport in undisturbed columns of weathered fractured shale. American Society of Agronomy. Anaheim, CA.

Mayes, M. A., Reedy, O. C., Larsen, I. L., Brooks, S. C., & Jardine, P. M. (1997, Oct.). Multispecies contaminant transport in undisturbed columns of weathered fractured shale. Geologic Society of America.

Mehlhorn, T. L., Jardine, P. M., Brooks, S. C., Fendorf, S. E., & Saiers, J. E. (1997, Oct. 26-31). Geochemical processes governing the fate and transport of Cr(III) and Cr(VI) in soils. American Society of Agronomy. Anaheim, CA.

Sanford, W. E., & Jardine, P. M. (1997, Oct. 26-31). Examining diffusion with multiple tracers to aid remediation of contaminated sites. American Society of Agronomy. Anaheim, CA.

Zhang, C., Brooks, S., Fendorf, S., & Jardine, P. (1998, Aug.). Microbial uranium reduction and biomineralization: Implication for immobilization of toxic metals and radionuclides. 17th Annual Meeting of the International Mineralogical Association. Toronto, Ontario, Canada.

Publication Type: Press release

Evans, R. & Hill, D. (1999). Press release initated by Department of Energy. One of 5 out of 200 EMSP projects to be featured in a press release package.

Norton, D. (1999, summer). Building a wall of bacteria. Initiatives in Environmental Technology Investment. Publication of the Waste Policy Institute. Blacksburg, VA. 6.

Publication Type: Proceeding

Fendorf, S. E., Jardine, P. M., Taylor, D. L., & Brooks, S.C. (1999). Auto-inhibition of oxide mineral oxidative capacity toward Co(II)EDTA: Time-resolved studies using XANES spectroscopy. Sparks, D. L. & Grundel, T. (Eds.), Kinetics and mechanisms of sorption processes at the mineral-water interface. ACS Symposium Series. 715, 358-371.

Jardine, P. M. (1998, Aug. 24-28). Can basic research on contaminant transport be used to improve the design of remedial strategies? Proceedings of “School of Environmental Science and Technology”. Buenos Aires, Argentina.

Jardine, P. M. (1998, Dec. 31). Auto-inhibition of oxide mineral oxidation capacity toward Co(II) EDTA: Time-resolved studies using XANES spectroscopy. Sparks, D. L., & Grundel, T. (Eds.), Kinetics and mechanisms of sorption processes at the mineral-water interface. ACS Symposium Series.

Publication Type: Theses/Dissertations

Bostick, B. (1997). Pyrite chemistry in soils and waters: Reactivity toward radionuclides and heavy metals. Master’s Thesis. Soil Science, University of Idaho. Moscow, ID.

Bostick, B. (Projected 2001). Sulfide and carbonate mineral adsorption processes of oxo-ions. Ph. D. candidate. Geological and Environmental Sciences, Stanford University. Palo Alto, CA.

Guha, H. (2000). Development and evaluation of a mathematical model for evaluating time-dependent hydrologic-biogeochemical processes at contaminated sites. M. S. Thesis, Florida International University.

Patterson, R. R. (1996). Iron sulfide reduction of chromate. Master's Thesis. Soil Science, University of Idaho. Moscow, ID.

Engineering Science

Project: 70088

Title: Interfacial Reduction-Oxidation Mechanisms Governing Fate and Transport of Contaminants in the Vadose Zone

PI: Dr. Baolin Deng *Institution:* University of Missouri at Columbia

Publication Type: Journal

Kim, C., Zhou, Q., Deng, B., Thornton, E. C., & Xu, H. (2001, in press). Chromium(VI) reduction by hydrogen sulfide in aqueous media: Stoichiometry and kinetics. Environmental Science and Technology.

Publication Type: Poster

Thornton, E. C., et. al. (2000). Interfacial reduction-oxidation mechanisms governing fate and transport of contaminants in the vadose zone. EMSP National Workshop 2000. Atlanta, GA.

Zhou, Q., Kim, C., Deng, B., & Thornton, E. C. (2000, Aug. 20-24). Effects of mineral surfaces on chromium(VI) reduction by hydrogen sulfide. The 220th ACS National Meeting. Washington, D. C.

Publication Type: Presentation

Kim, C., Lan, Y., Deng, B., & Thornton, E. C. (2001, Apr. 1-5). Catalytic effects of goethite on chromium(VI) reduction by hydrogen sulfide in anaerobic aqueous phase. 221st ACS National Meeting. San Diego, CA.

Kim, C., Zhou, Q., Deng, B., & Thornton, E. C. (2000, Aug. 20-24). Chromium(VI) reduction by hydrogen sulfide in the aqueous phase. The 220th ACS National Meeting. Washington, D. C.

Lan, Y., Kim, C., Deng, B., & Thornton, E. C. (2001, Apr. 1-5). Chromium(VI) reduction by sulfide under anaerobic conditions: Catalysis of elemental sulfur product. 221st ACS National Meeting. San Diego, CA.

Thornton, E. C., et. al. (1999). Laboratory evaluation of surface-catalyzed reduction mechanisms in the H2S-O2-Cr(VI)-sediment system. Geological Society of America Annual Meeting. Denver, CO.

Project: 73793 (Renewal of Project No. 55013)

Title: Biofiltration of Volatile Pollutants: Solubility Effects

PI: Dr. Brian H. Davison *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Barton, J. W., Davison, B. H., Klasson, K. T., & Gable III, C. C. (1999). Estimation of mass transfer and kinetics in operating trickle-bed bioreactors for removal of VOCs. Environmental Progress. 18, 87-92.

Barton, J. W., Hartz, S. M., Klasson, K. T., & Davison, B. H. (1997). Microbial removal of alkanes from dilute gaseous waste streams: Mathematical modeling of advanced bioreactor systems. J. Chem. Technol. Biotechnol. 72, 93-98.

Barton, J. W., Klasson, K. T., & Davison, B. H. (1997). Microbial removal of alkanes from dilute gaseous waste streams: Kinetics and mass transfer considerations. Biotechnology Progress. 13, 814-821.

Davison, B. H., Barton, J. W., Klasson, K. T., & Francisco, A. B. (2000, May 5). The influence of high biomass concentrations on alkane solubities. Biotechnology and Bioengineering, 68(3), 279-284.

Publication Type: Presentation

Barton, J. W. (1998, Jul.). Fundamental mechanisms for improved design, long-term operation, prediction, and implementation. EMSP Review Meeting. Chicago, IL.

Barton, J. W. (2000). Fundamental mechanisms for improved design, long-term operation, prediction, and implementation. EMSP Review Meeting, Atlanta, GA.

Barton, J. W., Davison, B. H., Klasson, K. T., Gable, III, C. C. (1997, Nov.). Estimation of mass transfer and kinetics in operating biofilters for removal of VOC's. AICHE Annual Meeting. Los Angeles, CA.

Barton, J. W., Klasson, K, T., & Davison, B. H. (1997, Aug. 6-8). Extended performance and evaluation of trickle bed bioreactors designed for VOC removal. Southern Section Annual Meeting of the Air & Waste Management Association. Gaitlinburg, TN.

Barton, J. W., Zhang, X. S., Klasson, K. T., & Davison, B. H. (1998). Predictive mathematical modeling of trickling bed biofilters for elucidating mass transfer and kinetic effects. Presented at the Air & Waste Management Association's 91st Annual Meeting & Exhibition. San Diego, CA.

Davison, B. H. (1999, Mar. 23). Effect of biomass on the measured solubility of sparingly soluble organics in aqueous bioremediation systems. The 217th American Chemical Society Meeting. Anaheim, CA.

Klasson, K. T., Barton, J. W., & Davison, B. H. (1999, Jun.). Performance of a propane-degrading bacterium. 92nd Annual Meeting of the Air and Waste Management Association. St. Louis, MO.

Klasson, K. T., Davison, B. H., Barton, J. W., Just, E. M., & Gable, II, C. C. (1997, Sep.). Biofiltration of chlorinated and non-chlorinated alkanes. Platform presentation at the American Chemical Society's Emerging Technologies in Hazardous Waste Management IX (Enviro Expo '97). Pittsburgh, PA.

Publication Type: Proceeding

Barton, J. W., Klasson, K. T., & Davison, B. H. (1997). Extended operation and control of biomass overgrowth in biofilters designed for VOC removal. Proceedings of the 90th Annual Meeting & Exhibition of Air & Waste Management Association. Toronto, Ontario, Canada.

Barton, J. W., Zhang, X. S., Klasson, K. T., & Davison, B. H. (1998, Jun.). Predictive mathematical modeling of trickling bed biofilters for elucidating mass transfer and kinetic effects. Proceedings of the 91st Annual Meeting of the Air & Waste Management Association. San Diego, CA. Paper 98-WAA.13P.

Barton, J. W., Zhang, X. S., Klasson, K. T., & Davison, B. H. (1998, Oct. 23). Predictive mathematical modeling of trickling bed biofilters. Proceedings of the 1998 USC-TRG Conference on Biofiltration. Los Angeles, CA.

Klasson, K. T., Barton, J. W., & Davison, B. H. (1999, Jun.). Performance of a propane-degrading bacterium. Proceedings of the 92nd Annual Meeting of the Air and Waste Management Association. St. Louis, MO.

Klasson, K. T., Davison, B. H., Barton, J W., & Jacobs, J. E. (1998, Jun.). Removal of chlorinated and nonchlorinated alkanes in a trickling bed biofilter. Proceedings of the 91st Annual Meeting of the Air and Waste Management Association. San Diego, CA. Paper 98-WAA.06P.

Klasson, K. T., Davison, B. H., Barton, J. W., & Jacobs, J. E. (1998). Removal of chlorinated and non-chlorinated alkanes in a trickle-bed reactor. Proceedings of the 91st Annual Meeting of the Air & Waste Management Association. San Diego, CA.

Publication Type: Theses/Dissertations

DeLozier, G. C. (1998, Dec.). Isolation and identification of VOC metaolizing microorganisms from an active biotrickling filter. Master's Thesis, School of Biotechnology, University of Tennessee. Knoxville, TN.

Geochemistry

Project: 54548

Title: The Efficacy of Oxidative Coupling for Promoting In-Situ Immobilization of Hydroxylated Aromatics in Contaminated Soil and Sediment Systems

PI: Dr. Walter J. Weber, Jr. *Institution:* University of Michigan

Publication Type: Poster

Keinath, II, T. M., Selig, H., & Weber, Jr., W. J. (1998, Oct. 16-18). Enzyme catalyzed oxidative coupling: Effect of horseradish peroxidase additions on sorption of phenols on natural organic sorbents. 21st Midwest Environmental Chemistry Workshop. The Univeristy of Michigan. Ann Arbor, MI.

Keinath, II, T. M., Selig, H., Payne, C., Suh, J. W., & Weber, Jr., W. J. (1999, Aug. 21-25). Induced sequestration of phenolic compounds by natural sorbents via MnO2 and oxidoreductase enzymes by coupling: Comparison of equilibrium and non-equilibrium systems. 217th National Meeting of the American Chemical Society. New Orleans, LA.

Orlov, A., Bandhari, A., Selig, H., & Weber, Jr., W. J. (1998, Oct. 16-18). Sequestration of phenolic compounds in natural sorbents through abiotic oxidative coupling reactions: The role of organic matter composition. 21st Midwest Environmental Chemistry Workshop. The University of Michigan. Ann Arbor, MI.

Publication Type: Presentation

Huang, Q., Selig, H., Keinath, II, T. M., & Weber, Jr., W. J. (2000, Mar. 26-31). Horseradish peroxidase-catalyzed phenol coupling in the presence of soil: Effects of enzyme inactivation. 219th ACS National Meeting. San Francisco, CA.

Keinath, II, T. M., Selig, H., Taylor, M., Payne, C., & Weber, Jr., W. J. (2000, Mar. 5-9). Sequestration of phenolic compounds by natural sorbents via Birnessite induced oxidative coupling. 2000 Spring National Meeting of the American Institute of Chemical Engineers. Atlanta, GA.

Project: 54635

Title: Molecular-Level Process Governing the Interaction of Contaminants with Iron and Manganese Oxides

PI: Dr. Scott A. Chambers *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

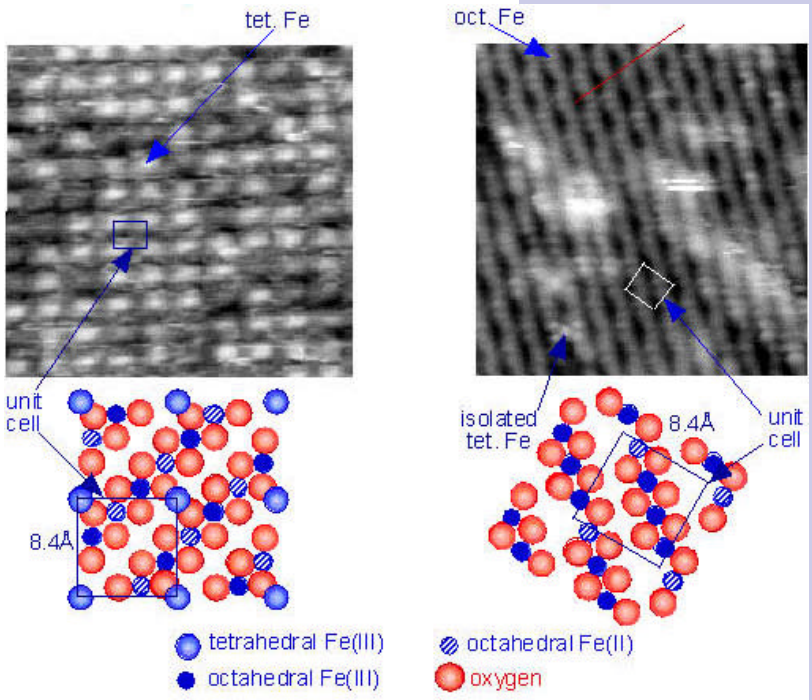
Brown, G. E. Jr., et. al. (1999). Metal oxide surfaces and their interactions with aqueous solutions and microbial organisms. Chem. Rev. 99, 77-174.

Chambers, S. A. & Liang, Y. (1999). Growth of • -MnO2 films on TiO2(110) by oxygen-plasma-assisted molecular beam epitaxy. Surf. Sci. Spect. 420, 123.

Chambers, S. A., & Joyce, S. A. (1999). Surface termination, composition, and reconstruction of Fe3O4(001) and • -Fe2O3(001). Surf. Sci. Spect. 420, 111.

Chambers, S. A., Gao, Y. & Kim, Y. J. (1998). Fe 2p core-level spectra for pure, epitaxial • -Fe2O3(0001), • -Fe2O3(001), and Fe3O4(001). Surf. Sci. Spect. 5, 219.

Foster, N. S., Amonette, J. E., & Autrey, S. T. (1999, Jun.). In situ detection of chromate using photoacoustic spectroscopy. Appl. Spectrosc. 53(6), 735-740.



Left: Top layer consists of tetrahedrally coordinated Fe(III), as shown in the structural diagram. Right: Top layers consist of octahedrally coordinated Fe(II) and Fe(III), along with tetrahedrally coordinated O, as shown in the structural diagram. [see Project #54635]

Foster, N. S., Autrey, S. T., Amonette, J. E., Small, J. R., & Small, E. W. (1999). Laser photoacoustic spectroscopy: A versatile absorption spectroscopic technique. Am. Lab. 31, 96s-108s.

Grolimund, D., et. al. (1999, May 1). Identification of Cr species at the aqueous solution-hematite interface after Cr(VI)-Cr(III) reduction using GI-XAFS and Cr L-edge NEXAFS. J. Synchrotron. Radiat. 6, 612-614, Part 3.

Kendelewicz, T., et. al. (1999). X-ray absorption and photoemission study of the adsorption of aqueous Cr(VI) on single crystal hematite and magnetite surfaces. Surf. Sci. Spect. 424, 219.

Kendelewicz, T., Liu, P., Brown, G. E. Jr., Nelson, E. J., & Chambers, S. A. (1999). Reaction of water with the (100) and (111) surfaces of Fe3O4. Surface Science.

Li, S. I., et. al. (1999, Dec. 20). Morphological and structural investigation of the early stages of epitaxial growth of alpha-Fe2O3 (0001) on alpha-A12O3 (0001) by oxygen-plasma-assisted MBE. Surf. Sci. 443(3), 212-220.

Liu, P., Kendelewicz, T., Brown, G. E. Jr., Nelson, E. J. & Chambers, S. A. (1998). Reaction of water vapor with • -Al2O3(0001) and • -Fe2O3(0001) surfaces: Synchrotron x-ray photoemission studies and thermodynamic calculations. Surf. Sci. Spect. 417, 53.

Rustad, J. R., Dixon, D. A., Kubicki, J. D., & Felmy, A. R. (2000, May 4). Gas-phase acidities of tetrahedral oxyacids from ab initio electronic structure theory. J. Phys. Chem. A. 104(17), 4051-4057.

Rustad, J. R., Wasserman, E., & Felmy, A. R. (1999, Jul. 9). A molecular dynamics investigation of surface reconstruction on magnetite (001). Surf. Sci. 432(1-2), L583-L588.

Thevuthasan, S., et. al. (1999). Surface structure of MBE-grown • -Fe2O3(0001) by intermediate-energy x-ray photoelectron diffraction. Surf. Sci. Spect. 425, 276-286.

Yi, S. I., Liang, Y. & Chambers, S. A. (1999). Effect of growth rate on the nucleation of • -Fe2O3 on • -Al2O3(0001) by oxygen-plasma-assisted molecular beam epitaxy. J. Vac. Sci. Technol. A.

Publication Type: Presentation

Amonette, J. E., Foster, N. S., William, B. K., & Taylor, A. E. (1999, Mar. 21-25). Trace-level chromate sorption dynamics at hematite surfaces: A spectroscopic approach. 217th National Meeting of the American Chemical Society. Anaheim, CA.

Amonette, J. E., Foster, N. S., William, B. K., & Taylor, A. E. (1999, Jun.). Competitive trace-level sorption of chromate and phosphate to hematite surfaces: A spectroscopic approach. 36th Annual Meeting of the Clay Minerals Society. Purdue University. West Lafayette, IN.

Brown, G. E. Jr., et. al. (1999, Mar.). Characterization of adsorbed chemical species at mineral surfaces. 217th American Chemical Society Meeting. Anaheim, CA.

Chambers, S. A. (1998, Oct.). Molecular beam epitaxial growth and surface structure determination of Fe and Mn oxides. Invited presentation at the Center for Catalysis and Surface Structure. Northwestern University. Evanston, IL.

Chambers, S. A., Thevuthasan, S., Kim, Y. J., Joyce, S. A., & Liang, Y. (1998, Aug.). Surface structure determination of MBE grown iron and manganese oxides. Invited presentation at the National Meeting of the American Chemical Society. Boston, MA.

Chambers, S. A.,Thevuthasan, S., & Joyce, S. A. (1999, Jan.). Structure and reactivity of MBE-grown Fe oxides. Invited presentation at the First International Conference on Oxide Surfaces. Elmau, Germany.

Grolimund, D., et. al. (1998, Jul.). Identification of Cr species at the solution-hematite interface after Cr(VI)-Cr(III) reduction using GI-XAFS and Cr L-edge NEXAFS. 10th International XAFS Conference. Chicago, IL.

Grolimund, D., Fitts, J. P., Trainor, T. P., Brown, G. E. Jr., & Chambers, S. A. (1999, Mar.). Identification of Cr species at the aqueous solution-oxide interface using grazing-incidence XAFS. 217th American Chemical Society Meeting. Anaheim, CA.

Joyce, S. A., Thevuthasan, S., & Chambers, S. A. (1999, Mar. 21-25). Growth and structure of synthetic iron oxide mineral surfaces. 217th National Meeting of the American Chemical Society. Anaheim, CA.

Kendelewicz, T., Liu, P., Brown, G. E. Jr., & Nelson, E. J. (1998, Aug.). Reaction of water with (100) and (111) surfaces of magnetite (Fe3O4). International Conference on Surface Science 10. Birmingham, United Kingdom.

Kendelewicz, T., Liu, P., Brown, G. E. Jr., Chambers, S. A., & McCarthy, M. I. (1998, Aug.). “Hydroxylation of the surfaces of simple metal oxides: Spectroscopic and thermodynamic analysis. Goldschmidt Conference. Toulouse, France.

Kendelewicz, T., Liu, P., Brown, G. E. Jr., Nelson, E. J., & Chambers, S. A. (1998, Aug.). Reduction of the (0001) surface of hematite (• -Fe2O3) prepared under UHV conditions. International Conference on Surface Science 10. Birmingham, United Kingdom.

Kendelewicz, T., Liu, P., Brown, G. E. Jr., Nelson, E. J., & Chambers, S. A. (1998, Aug.). Fe L2,3 and O K near edge structure of iron oxides and hydroxides. International Conference on Surface Science 10. Birmingham, United Kingdom.

Kendelewicz, T., Liu, P., Brown, G. E. Jr., Nelson, E. J., & Chambers, S. A. (1998, Aug.). Reaction of water with clean (0001) and (1-102) surfaces of • -Fe2O3. International Conference on Surface Science 10. Birmingham, United Kingdom.

McCready, D. E., (1998, Jun.). Rutherford backscattering and channeling studies of epitaxially grown iron oxide films on various substrates. Surface Analysis/8th Annual Pacific Northwest Symposium.

Rustad, J. R. (1999, Aug.). Molecular simulation of the iron oxide-water interface. Invited presentation at the American Chemical Society Meeting. New Orleans, LA.

Rustad, J. R., Wasserman, E., & Joyce, S. A. (1999, Mar. 21-25). Structure and energetics of the magnetite(001) surface insights from molecular dynamics calculations. 217th National Meeting of the American Chemical Society. Anaheim, CA.

Thevuthasan S. (1998, Nov.). Rutherford backscattering and channeling studies of Al and Mg diffusion in iron oxide thin films. Invited presentation at the Fifteenth International Conference on the Application of Accelerators. Denton, TX.

Thevuthasan, S., et. al. (1998, Jun.). The surface structure determination of • -Fe2O3 by intermediate-energy x-ray photoelectron diffraction. Surface Analysis/8th Annual Pacific Northwest Symposium.

Thevuthasan, S., et. al. (1998, Nov.). The surface structure determination of • -Fe2O3 (0001) by low-energy x-ray photoelectron diffraction. 45th National Symposium of the American Vacuum Society.

Thevuthasan, S., Jiang, W., McCready, D. E., & Chambers, S. A. (1998, Nov.). Rutherford backscattering and channeling studies of Al and Mg diffusion in iron oxide thin films. 45th National Symposium of the American Vacuum Society.

Thevuthasan, S., McCready, D. E., Jiang, W., Yi, S. I., & Chambers, S. A. (1999, Jul.). Ion beam analysis of interface reactions in iron oxide thin films. Invited presentation at the Fourteenth International Conference on Ion Beam Analysis (IBA-14). Dresden, Germany.

Publication Type: Proceeding

Chambers, S. A., & Liang, Y. (1998, Nov.). Growth of • -MnO2 films on TiO2(110) by oxygen-plasma- assisted molecular beam epitaxy. 45th International Symposium of the American Vacuum Society. Baltimore, MD.

Project: 54741

Title: Characterization of Contaminant Transport Using Naturally-Occurring U-Series Disequilibria

PI: Dr. Michael T. Murrell *Institution:* Los Alamos National Laboratory

Publication Type: Journal

Ku, T. L., Luo, S., Leslie, B. W., & Hammond, D. E. (1998). Assessing radionuclide migration from natural analog studies: Response to McKinley and Alexander (1996). Radiochimica Acta 80. 219-223.

Luo, S., Ku, T. L., Roback, R., Murrell, M., & McLing, T. L. (2000). In-situ radionuclide transport and preferential groundwater flows at INEEL (Idaho): Decay-series disequilibrium studies. Geochimica et Cosmochimica Acta, 64, #3.

Publication Type: Presentation

Luo, S., Ku, T. L., Roback, R., Murrell, M., & McLing, T. L. (1999, Nov. 29 - Dec. 3). Decay-series disequilibrium study of in-situ, long-term radionuclide transport in water-rock systems. MRS 1999 Fall Meeting Abstract Volume, Boston, MA. 734.

Luo, S., Ku, T. L., Roback, R., Murrell, M., & McLing, T. (1999, Aug. 21-26). Uranium-series disequilibria in groundwater: Assessing radionuclide migration. 9th International Conference on Isotope Geology, Cosmochemistry and Geochronology. Beijing, China.

Murrell, M. & Ku, T. L. (1998, Jul. 27-30). Characterization of contaminant transport using naturally occurring U-series disequilibria. DOE Environmental Management Science Program Workshop, Rosemont, IL. CONF-980736, Poster 179, 358-359.

Publication Type: Proceeding

Luo, S., Ku, T. L., Roback, R., Murrell, M., & McLing, T. L. (2000). Decay-series disequilibrium study of in-situ, long-term radionuclide transport in water-rock systems. Proceedings on Scientific Basis for Nuclear Waste Management XXIII, Material Research Society.

Luo, S., Ku, T. L., Roback, R., Murrell, M., & McLing, T. (1998, Dec. 6-10). Assessing in-situ radionuclide transport based on uranium-series disequilibrium in groundwater. Fall AGU Meeting. San Francisco, CA. EOS Trans. Amer. Geophys. Un. 79, F354.

Roback, R. C., et. al. (1997). Groundwater mixing, flow-paths and water/rock interaction at INEEL: Evidence from uranium isotopes. Geological Society of America, Abstracts with Programs. 29(6).

Roback, R. C., et. al. (1998, Dec. 6-10). Uranium and thorium series isotopes in fractured rocks at the INEEL. Fall AGU Meeting. San Francisco, CA. EOS Trans. Amer. Geophys. Un. 79, F343.

Project: 54823

Title: Modeling of Cation Binding in Hydrated 2:1 Clay Minerals
PI: Dr. David E. Smith *Institution:* New Mexico State University

Publication Type: Journal

Shroll, R. M. & Smith, D. E. (1999). Molecular dynamics simulations in the grand canonical ensemble: Application to clay mineral swelling. J. Chem. Phys. 111, 9025.

Shroll, R. M. & Smith, D. E. (1999). Molecular dynamics simulations in the grand canonical ensemble: Formation of a bias potential for umbrella sampling. J. Chem. Phys. 110, 8295.

Smith, D. E. (1998). Molecular computer simulations of the swelling properties and interlayer structure of cesium montmorillonite. Langmuir. 14, 5959.

Young, D. A. & Smith, D. E. (2000). Simulations of clay mineral swelling and hydration: Dependence upon interlayer ion size and charge. J. Phys. Chem. B. 104, 9163.

Project: 55014

Title: Kinetics and Mechanisms of Metal Retention/Release in Geochemical Processes in Soil

PI: Dr. Robert W. Taylor *Institution:* Alabama A&M University

Publication Type: Journal

Shen, S. Y., Taylor, R. W., Bart, H., & Tu, S. (1999). Equilibrium and spectroscopic studies of lead retention in smectite. Commun. Soil Sci. Plan. 30(19-20), 2711-2730.

Shen, S., Taylor, R. W., Bart, H., & Tu, S. I. (1999). Equilibrium and spectroscopic studies of lead retention in smectite. Commun. Soil Sci. Plant Anal. 30(19-20), 2711-2730.

Taylor, R. W., Shen, S., Bleam, W. F., & Tu, S. I. (2000, in press). Chromate removal by dithionite-reduced clays: Direct XANES evidence of chromate reduction at clay surfaces. Clays Clay Min.

Xia, K., Bleam, W. F., & Helmke, P. A. (1997). Studies of the nature of binding sites of first row transition elements bound to aquatic and soil humic substances using x-ray absorption spectroscopy. Geochim. Cosmochim. Acta. 61, 2223-2235.

Xia, K., Bleam, W. F., & Helmke, P. A. (1997). Studies of nature of Cu2+ and Pb2+ binding sites in soil humic substances using X-ray absorption spectroscopy. Geochim. Cosmochim. Acta. 61, 2211-2221.

Xia, K., et. al. (1998). XANES studies of oxidation states of sulfur in aquatic and soil humic substances. Soil Sci. Soc. Am. J. 62, 1240-1246.

Metal Retention/Release Mechanisms for Geochemical Soil Processing. [see Project #55014]

Xia, K., Mehadi, A., Taylor, R. W., & Bleam, W. F. (1997). X-ray absorption and electron paramagnetic resonance studies of Cu(II) sorbed to silica: Surface-induced precipitation at low surface covergaes. J. Colloid Interface Sci. 185, 252-257.

Xia, K., Skylberg, U. L., Bleam, W. F., & Bloom, P. R. (1999). X-ray absorption spectroscopic evidence for the complexation of Hg(II) by reduced sulfur in soil humic substances. Environ. Sci. Technol. 33, 257-261.

Xia, K., Taylor, R. W., Bleam, W. F., & Helmke, P. A. (1998). The distribution of Cu(II) on boehmite and silica surfaces: Correlating EPR signal loss with the effective Bohr magnetron number of sorbed soils. J. Colloid Interface Sci. 199, 77-82.

Publication Type: Presentation

Bleam, W. (1999). Humic substances in geochemical processes: Metal complexation, redox reaction, and sorption of non-polar organic compounds. Environmental Molecular Sciences Symposium and First EMSL Users Meeting. Pacific Northwest National Lab. Richland, WA.

Bleam, W. F. (1998). Nano-mineralogy and the chemistry of trace elements in soils. Presentation at Kansas State University. Manhattan, KS.

Bleam, W. F. (1998). Recent developments in metal complexation by humic substances, 10/24/98. Natural Organic Matter Research in Soils and Water. International Humic Substances Society Workshop. University of Minnesota. St. Paul, MN.

Bleam, W. F., et. al. (1998). Recent advances in understanding the chemistry of Cr(VI), Pb(II) and Hg(II) in soils: Adsorption to mineral surfaces and complexation by humic substances. Agronomy Abstracts. Baltimore, MD. 36.

Bleam, W. F., Yoon, S. J., Szulczewski, M. A., Martinez, C. E., & Shen, S. (1998). Environmental chemistry at NSLS, 1998. National Synchrotron Light Source. Brookhaven National Laboratory. Upton, NY.

Ranatunga, T. D., Taylor, R. W., Bleam, W. F., & McWhinney, H. G. (2000). Lead adsorption on Kaolinite. Annual Meeting. Soil Science Society of America. Minneapolis, MN.

Shen, S., Taylor, R. W., & Tu, S. I. (1997). Equilibrium and Spectroscopic Studies of Lead Retention in Smectite. Argonomy Abstracts. Anaheim, CA. 190.

Shen, S., Taylor, R. W., Bleam, W. F., & Tu, S. I. (1998). Coupled reduction-sorption of chromate in dithionite-reduced smectites. Agronomy Abstracts. Baltimore, MD. 189.

Szulczewski, M. D., Xia, K., Helmke, P. A., Bleam, W. F., & Taylor, R. W. (1998). Evaluating the reductive capacity of humic substances: Reactions between thiol/thio groups and chromate. Agronomy Abstracts, Baltimore, MD. 38.

Taylor, R. W., Shen, S., Bleam, W. F., & Tu, S. (1999, Jul. 11-15). Chromate removal by dithionite-reduced clays. 5th International Conference on the Biogeochemistry of Trace Elements. Vienna, Austria.

Project: 55148

Title: Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry

PI: Dr. Gregory Nimz *Institution:* Lawrence Livermore National Laboratory

Publication Type: Journal

McAninch, J. E., et. al. (1998). Detection of 99Tc by accelerator mass spectrometry: Preliminary investigations. J. Radioanal. Nucl. Chem. 234, 125-129.

Publication Type: Proceeding

Caffee, M. W., Nimz, G. J., & Roberts, M. L. (1999). Measurement of iodine-129 in unsaturated soils: Transport properties and distribution of iodine-129 in depth profiles. EOS: Transactions of the American Geophysical Union, AGU Fall Meeting, San Francisco, CA.

Project: 55249

Title: Experimental Determination of Contaminant Metal Mobility as a Function of Temperature, Time, and Solution Chemistry

PI: Dr. Susan A. Carroll *Institution:* Lawrence Livermore National Laboratory

Publication Type: Journal

Sahai, N., Carroll, S. A., Roberts, S. & O'Day, P. A. (2000). X-ray absorption spectroscopy of strontium (II) coordination. II. Sorption and precipitation at kaolinite, silica gel, and goethite surfaces. J. Colloid and Interface Science. 222, 198-212.

O'Day, P. A., Newville, M., Neuhoff, P. S., Sahai, N., & Carroll, S. A. (2000). X-ray absorption spectroscopy of strontium (II) coordination. I. Static and thermal disorder in crystalline, hydrated, and precipitated solids and in aqueous solution. J. Colloid and Interface Science. 222, 184-197.

Project: 55284

Title: Aquifer Transport of Th, U, Ra, and Rn in Solution and on Colloids

PI: Dr. G. J. Wasserburg *Institution:* California Institute of Technology

Publication Type: Journal

Tricca, A., Porcelli, D., Wasserburg, G. J., & Baskaran, M. (1998). Transport of U- and Th-series radionuclides in groundwater. 8th Vv. M. Goldschmidt Conference. Toulouse, France. Mineralogical Magazine. 62A, 1543-1544.

Tricca, A., Porcelli, D., Wasserburg, G. J., & Baskaran, M. (2001, in press). Transport of U- and Th-series radionuclides in a sandy aquifer. Geochim. Cosmochim. Acta.

Tricca, A., Porcelli, D., Wasserburg, G. J., Baskaran, M., & Naidu, J. (1998). Development of a transport model of U-Th decay series nuclides in groundwater and its application to a sandy aquifer. Eos Trans. Amer. Geophys. U. 79, F425.

Publication Type: Presentation

Tricca, A., Porcelli, D., Wasserburg, G. J., & Baskaran, M. (2000, Apr.). Transport of U- and Th-series radionuclides in a sandy aquifer. DOE Conference. Atlanta, GA.

Project: 70070

Title: Reactivity of Primary Soil Minerals and Secondary Precipitates Beneath Leaking Hanford Waste Tanks

PI: Dr. Kathryn L. Nagy *Institution:* University of Colorado

Publication Type: Presentation

Gamerdinger, A. P., Kaplan, D. I., & Serne, R. J. (2000, Dec. 15-19). Effect of mobile-immobile water on uranium sorption during transport in unsaturated sand-textured sediments. AGU Fall Meeting. San Francisco, CA.

Kaplan, D. I., Gamerdinger, A. P., & Serne, R. J. (2000, Dec. 15-19). Effect of rate-limited sorption on uranium mobility in unsaturated silt-textured sediments. AGU Fall Meeting. San Francisco, CA.

Serne, R. J., Last, G. V., Myers, D. A., & Sobczyk, S. M. (2000, Dec. 15-19). Results and interpretation from Hanford's SX tank farm vadose sediment sampling. AGU Fall Meeting. San Francisco, CA.

Sobczyk, S. M. & Serne, R. J. (2000, Dec. 15-19). Subsurface interpretation of the SX tank farm, Hanford site, Washington, based on gamma-ray logging. AGU Fall Meeting. San Francisco, CA.

Steefel, C. I., Lichtner, P. C., Yabusaki, S. B., Pruess, K. L., & Serne, R. J. (2000, Dec. 15-19). I: Cesium migration in Hanford sediments below leaking HLW tanks. AGU Fall Meeting. San Francisco, CA.

Yabusaki, S. B. (2000, Dec. 15-19). Radioactive and mixed waste in the vadose zone: Characterization, experimental studies, and modeling. Special Session on Hanford Vadose Zone, AGU Fall Meeting. San Francisco, CA.

Project: 70163

Title: The Aqueous Thermodynamics and Complexation Reactions of Anionic Silica Species to High Concentration: Effects on Neutralization of Leaked Tank Wastes and Migration of Radionuclides in the Subsurface

PI: Dr. Andrew R. Felmy *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Felmy, A. R., Cho, H., Rustad, J. R., & Mason, M. J. (2001, in press). An aqueous thermodynamic model for polymerized silica species to high ionic strength. J. Solution Chem.

Publication Type: Presentation

Felmy, A. R., Cho, H., Rustad, J. R., Dixon, D. A., & Choppin, G. R. (2000, Nov. 28). The aqueous thermodynamics and complexation reactions of anionic silica species to high concentration. EMSP Principal Investigator Workshop. Richland, WA.

Felmy, A. R., et. al. (2001). The aqueous complexation of Eu(III) with organic chelates at high base concentration: Molecular and thermodynamic modeling results. Nuclear Site Remediation - First Accomplishments of the Environmental Management Science Program. ACS Symposium Series 778, 5.

Felmy, A. R., et. al. (2001, Mar. 12-15). Development of accurate chemical models for tank waste applications. Tanks Focus Area Mid-Year Review. Salt Lake City, UT.

Project: 73745 (Renewal of Project No. 54585)

Title: Permanganate Treatment of DNAPLs in Reactive Barriers and Source Zone Flooding Schemes

PI: Dr. Frank W. Schwartz *Institution:* Ohio State University

Publication Type: Journal

Seol, Y. & Schwartz, F. W. (2000). Phase-transfer-catalyst applied to the oxidation of nonaqueous phase trichloroethylene by potassium permanganate. J. of Contaminant Hydrology. 44(2), 185-201.

Yan, Y. E. & Schwartz, F. W. (1999). Oxidative degradation and kinetics of chlorinated ethylenes by potassium permanganate. Journal of Contaminant Hydrology. 37(3-4), 343-365.

Yan, Y. E., & Schwartz, F. W. (2000). Kinetics and mechanisms for TCE oxidation by permanganate. Environmental Science and Technology. 34, 2535-2541.

Zhang, H., & Schwartz, F. W. (2000). Simulating the in situ oxidative treatment of chlorinated ethylenes by potassium permanganate. Water Resources Research. 36(10), 3031-3042.

Publication Type: Proceeding

Ibaraki, M. & Schwartz, F. W. (2000, May 22-25). On source-zone flooding for treating DNAPL sites. Treating Dense Nonaqueous Phase Liquids (DNAPLs). The Second International Conference on Remediation of Chlorinated and Recalcitrant Compounds. Monterey, CA. 2(6), 125-132.

Li, X. & Schwartz, F. W. (2000, May 22-25). Efficiency problems related to permanganate oxidation schemes. Chemical Oxidation and Reactive Barriers. The Second International Conference on Remediation of Chlorinated and Recalcitrant Compounds. Monterey, CA. 2(6), 41-48.

Seol, Y. & Schwartz, F. W. (2000, May 22-25). Phase-transfer-catalysis on the oxidation of trichloroethylene by permanganate. Chemical Oxidation and Reactive Barriers. The Second International Conference on Remediation of Chlorinated and Recalcitrant Compounds. Monterey, CA. 2(6), 17-24.

Yan, Y. E. & Schwartz, F. W. (1998, May 18-21). Oxidation of chlorinated solvents by permanganate. Physical, Chemical, and Thermal Technologies. The First International Conference on Remediation of Chlorinated and Recalcitrant Compounds. Monterey, CA. Battelle Press. Columbus, OH. 1(6), 403-408.

Zhang,H. & Schwartz, F. W. (2000, May 22-25). Simulation of oxidative treatment of chlorinated compounds by permanganate. Chemical Oxidation and Reactive Barriers. The Second International Conference on Remediation of Chlorinated and Recalcitrant Compounds. Monterey, CA. 2(6), 1-8.

Photographs of 3-D large tank experiment. The experiment was designed to simulate the in-situ remediation of TCE residually saturated in sand aquifer. Reaction occurring in the sand aquifer is subject to monitoring for concentration of TCE, permanganate and chloride as a reaction product. [see Project #73745, renewal of #54585]

Publication Type: Theses/Dissertations

Yan, Y. E. (1998). Abiotic remediation of ground water contaminated by chlorinated solvents. Ph D. Thesis. Ohio State University. Columbus, OH.

Project: 73758 (Renewal of Project No. 60355)

Title: Fixations Mechanisms and Desorption Rates of Sorbed Cs in High Level Waste Contaminated Subsurface Sediments: Implications to Future Behavior and In-Ground Stability

PI: Dr. John M. Zachara *Institution:* Pacific Northwest National Laboratory

Publication Type: Presentation

Zachara, J. M. (1999, Aug.). New advances in the understanding of 137Cs interactions with micas and implications to Cs geochemistry in the Hanford vadose zone. Keynote address given to the EMSP National Program Workshop. Chicago, IL.

Project: 73773 (Renewal of Project No. 55351)

Title: Isotopic Tracers for Waste Fluid Tracking and Fluid-Soil Interactions: Hanford, Washington

PI: Dr. Donald J. DePaolo *Institution:* Lawrence Berkeley National Laboratory

Publication Type: Journal

Geller, J. T., et. al. (2000). Flow dynamics and potential for biodegradation of organic contaminants in fractured rock vadose zone. J. Contaminant Hydrology. 33, 63-90.

Publication Type: Other

Conrad, M. E. & Faybishenko, B. (2001, in press). Isotopic tracers of flow and transport through the vadose zone. Looney, B. & Falta, R. (Eds.). Vadose Zone Technology and Science Solutions. Batelle Press. Columbus, OH.

Publication Type: Proceeding

Conrad, M. E., DePaolo, D. J., & Dresel, P. E. (2000). Natural isotopic tracers of infiltration through the vadose zone at the Hanford Site, Washington. Eos. Trans. Am. Geophys. Union. 81(19), S230.

Conrad, M. E., DePaolo, D. J., Kennedy, B. M., & Miller, E. C. (1997). Carbon isotope evidence for degradation of mixed contaminants in the vadose zone. Geol. Soc. Am. Abst. 26(6), A186.

Conrad, M. E., DePaolo, D. J., Song, D. L., & Neher, E. (1999). Isotopic evidence for groundwater flow and biodegradation of organic solvents at the Test Area North site, Idaho National Engineering and Environmental Laboratory. Ninth V. M. Goldschmidt Conference. 58-59. LPI Contribution No. 971. Lunar and Planetary Institute. Houston, TX.

Song, D. L., Alvarez-Cohen, L., Conrad, M. E., & Sorenson, K. (1999). Monitoring of enhanced in-situ bioremediation of trichloroethylene using stable carbon isotopes. Program and Abstracts for the 4th International Symposium on Subsurface Microbiology. Vail, CO.

Project: 73775 (Renewal of Project No. 55396)

Title: Colloid Genesis/Transport and Flow Pathway Alterations Resulting From Interactions of Highly Reactive Waste Solutions and Sediments in the Vadose Zone

PI: Dr. Jiamin Wan *Institution:* Lawrence Berkeley National Laboratory

Publication Type: Journal

Veerapaneni, S., Wan, J., & Tokunaga, T. K. (2000). Particle motion in film flow. Environ. Sci. & Technol. 34, 2465-2471.

Wan, J. & Tokunaga, T. K. (1998). Measuring partition coefficients of colloids at air-water interfaces. Environ. Sci. Technol. 32, 3293-3298.

Geophysics

Project: 54655

Title: Collaborative Research: Hydrogeological-Geophysical Methods for Subsurface Site Characterization

PI: Dr. Gary M. Mavko *Institution:* Stanford University

Publication Type: Presentation

Wempe, W. L. & Mavko, G. (1999, Oct.). The propagation of errors in Archie's water saturation equation: The influence of an a-m relationship. Presentation at the Geological Society of America 1999 Conference.

Publication Type: Proceeding

Corona, W. W. & Mavko, G. (1999, Mar.). Predicting clay content and porosity from gamma-ray and conductivity logs. SAGEEP Proceedings.

Wempe, W. L. & Mavko, G. (2000, Feb.). The electrical resistivity - acoustic velocity relationship: A method for constraining porosity. SAGEEP Proceedings.

Publication Type: Theses/Dissertations

Wempe, W. L. (2000). Predicting flow properties using geophysical data: Improving aquifer characterization. Ph.D. dissertation. Stanford University, Stanford, CA.

Project: 55011

Title: Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes

PI: Dr. James G. Berryman *Institution:* Lawrence Livermore National Laboratory

Publication Type: Journal

Berryman, J. G. (2000). Analysis of approximate inverses in tomography II. Iterative inverses. Optimization and Engineering, Volume 1, #1.

Berryman, J. G. (2000). Analysis of approximate inverses in tomography I. Resolution analysis of common inverses. Optimization and Engineering, Volume 1, #1.

Borcea, L., Berryman, J. G., & Papanicolaou, G. C. (1996). High contrast impedance tomography. Inverse Problems, 12, 835-858.

Borcea, L., Berryman, J. G., & Papanicolaou, G. C. (1999). Matching pursuit for imaging high contrast conductive media. Inverse Problems. 15, 811-849.

Dorn, O., Bertete-Aguirre, H., Berryman, J. G., & Papanicolaou, G. C. (1999, Dec. 19). A nonlinear inversion method for 3D-electromagnetic imaging using adjoint fields. Inverse Probl. 15(6), 1523-1558.

Publication Type: Patent

Berryman, J. G. (1998, Dec. 8). Robust discrimination of porosity and fluid saturation using seismic velocity analysis. Patent disclosure #IL-10437.

Berryman, J. G. (1998, Nov. 6). Joint inversion of electrical and electromagnetic tomography data for mapping saturation level and connectivity of conducting fluids underground. Patent disclosure#IL-10412.

Publication Type: Presentation

Berge, P. A. & Berryman, J. G. (1999, Mar. 24-27). Developing rock physics algorithms for velocity-porosity relations with environmental geophysics applications. Invited presentation at the Fifth SIAM Conference on Mathematical and Computational Issues in the Geosciences. San Antonio, TX.

Berryman, J. G. (1997, Aug. 25-29). Challenges for computational physics in underground imaging of electrically conducting contaminant plumes. Invited presentation P2.03 in special session on Geological Phenomena at the International Conference on Computational Physics. American Physical Society, Division of Computational Physics. Santa Cruz, CA.

Berryman, J. G. (1998, Oct. 19-23). Underground imaging of electrically conducting plumes. Invited presentation at the International Advanced Studies Institute, First International Symposium on Detection and Analysis of Subsurface Objects and Phenomena, Naval Postgraduate School. Monterey, CA.

Berryman, J. G., Berge, P. A. & Bonner, B. P. (1999, Nov. 4). Role of lambda-diagrams in estimating porosity and saturation from seismic velocities. Invited presentation at SEG, Houston, TX.

Publication Type: Proceeding

Berge, P. A., Berryman, J. G., Bonner, B. P., Roberts, J. J., & Wildenschild, D. (1999, Mar. 14-18). Comparing geophysical measurements to theoretical estimates for soil mixtures at low pressures. Invited presentation in the 1999 Conference Proceedings of the Symposium on the Application of Geophysics to Engineering and Environmental Problems (SAGEEP). Oakland, CA. 465-472.

Berge, P. A., Roberts, J. J., Berryman, J. G., & Wildenschild, D. (1998, Jul. 27-30). Joint inversion of geophysical data for site characterization and restoration monitoring. Abstract #188 in Proceedings of Environmental Sciences Management Workshop. Chicago, IL. 378-380.

Berryman, J. G. (1998, Jul. 27-30). Surface and borehole electromagnetic imaging of conducting contaminant plumes. Abstract #189 in Proceedings of Environmental Sciences Management Workshop. Chicago, IL. 380-382.

Berryman, J. G., Champagne II, N. J., & Buettner, H. M. (1999, Oct. 27-29). A 3D finite-difference frequency-domain code for electromagnetic induction tomography. Proceedings of the Second International Symposium on Three Dimensional Electromagnetics, University of Utah. Salt Lake City, UT.

Buettner, H. M. & Berryman, J. G. (1999, Mar. 14-18). An electromagnetic induction tomography field experiment at Lost Hills, CA. Invited presentation at the 1999 Conference Proceedings of the Symposium on the Application of Geophysics to Engineering and Environmental Problems (SAGEEP). Oakland, CA. 663-672.

Champagne II, N. J., Berryman, J. G., Buettner, H. M., Grant, J. B. & Sharpe, R. M. (1999, Mar. 14-18). A finite-difference frequency-domain code for electromagnetic induction tomography. Poster and paper in 1999 Conference Proceedings of the Symposium on the Application of Geophysics to Engineering and Environmental Problems (SAGEEP). Oakland, CA. 931-940.

Project: 55332

Title: A Hybrid Hydrologic-Geophysical Inverse Technique for the Assessment and Monitoring of Leachates in the Vadose Zone

PI: James R. Brainard *Institution:* Sandia National Laboratories - Albuquerque

Publication Type: Journal

Alumbaugh, D. L., Paprocki, L., Brainard, J., Glass, R. J., & Rautman, C. (2000, in press). Estimating in-situ moisture contents using cross-borehole ground penetrating radar; a study of accuracy, repeatability and resolution. Applied Geophysics.

Hughson, D. L. & Yeh, T. -C. J. (1998). A geostatiscally based inverse model for three-dimensional variably saturated flow. Stochastic Hydrology and Hydraulics. 12, 285-298.

Hughson, D. L. & Yeh, T. -C. J. (2000). An inverse model for three dimensional variably saturated flow. Water Resources Research. 36(4).

LaBrecque, D. J. & Yang, X. (2000, in press). Difference inversion of ERT data - a fast inversion method for 3-D in-situ monitoring. J. Environ. Eng. Geophys.

Li, B. & Yeh, T. -C. J. (1999). Cokriging estimation of the conductivity field under variably saturated flow conditions. Water Resour. Res. 35(12), 3663-3674.

Vargas-Guzman, J. A. & Yeh, T. -C. J. (1999). Sequential kriging and cokriging: Two powerful geostatistical approaches. Stochastic Environmental Research and Risk Assessment. 13(6), 416-435.

Publication Type: Presentation

Alumbaugh, D. & Paprocki, L. (2000). Monitoring infiltration within the vadose zone using cross-borehole ground penetrating radar. Proceedings of the Symposium on the Application of Geophysics for Environmental and Engineering Problems (SAGEEP). 273-281.

Brainard, J. R., et. al. (1999). Evaluation of geophysical and hydrologic measurements of an induced saturation field within heterogeneous deposits. Abstracts from the American Geophysical Union Annual Fall Meeting. San Francisco, CA.

LaBrecque, D. J., Yang, X., Alumbaugh, D. L., & Paprocki, L. (1999). Three-dimensional monitoring of vadose zone infiltration using ERT and cross-borehole ground penetrating radar. Proceedings of the Second International Symposium on Three-Dimensional Electromagnetics. Salt Lake City, UT. 329-332.

Paprocki, L. & Alumbaugh, D. (1999, Mar. 14-18). An investigation of cross-borehole ground penetrating radar measurements for characterizing the 2D moisture content distribution in the vadose zone. Proceedings of the Symposium on the Application of Geophysics to Environmental and Engineering Problems (SAGEEP) ’99. Oakland, CA. 583-592.

Yang, X. & LaBrecque, D. (1998, Mar. 22-26). 3-D stochastic inversion of ERT data. Proceedings of the Symposium on the Application of Geophysics to Environmental and Engineering Problems (SAGEEP) ’98. Chicago, IL. 221-228.

Yang, X. & LaBrecque, D. (2000, Feb. 20-24). Estimation of 3-D moisture content using ERT data at the Socorro infiltration site. Proceedings of the Symposium on the Application of Geophysics for Environmental and Engineering Problems (SAGEEP) ’00. Arlington, VA.

Yang, X. & LaBrecque, D. (2000, Feb. 20-24). Three-dimensional complex resistivity tomography. Proceedings of the Symposium on the Application of Geophysics for Environmental and Engineering Problems (SAGEEP) ’00. Arlington, VA.

Yeh, T. -C. J., Alumbaugh, D., Liu, S., & Paprocki, L. (1998). A stochastic hydrogeophysical joint inversion technique for monitoring and characterizing the vadose zone. AGU Fall Meeting 1998. San Francisco, CA.

Yeh, T. -C. J., LaBrecque, D., Alumbaugh, D., Li, B., & Yang, X. (1997). A stochastic hydrogeophysical joint inversion technique for monitoring movement of water and characterizing the vadose zone. AGU Fall Meeting 1997. San Francisco, CA.

Publication Type: Proceeding

Yang, X. & LaBrecque. (1999, Mar. 14-18). Comparison between stochastic and Occam’s inversion of 3-D ERT data. Proceedings of the Symposium on the Application of Geophysics to Environmental and Engineering Problems (SAGEEP) ’99. Oakland, CA. 979-988.

Publication Type: Report

Brainard, J. R., et. al. (2000, in press). The Sandia-tech vadose zone facility: Experimental design and data report of a constant flux infiltration experiment. Sandia National Laboratories.

Publication Type: Theses/Dissertations

Paprocki, L. T. (2000). Characterization of vadose zone in-situ moisture content and an advancing wetting front using cross-borehole ground penetrating radar. Master’s Thesis. Department of Hydrology, New Mexico Institute of Mining and Technology. Socorro, New Mexico.

Yang, X. (1999). Stochastic inversion of 3-D ERT data. Ph. D. dissertation. Department of Mining and Geological Engineering, University of Arizona. Tucson, AZ.

Project: 60162

Title: Enhancements to & Characterization of the Very Early Time Electromagnetic (VETEM) Prototype Instrument & Applications to Shallow Subsurface Imaging at Sites in the DOE Complex

PI: Dr. David L. Wright *Institution:* U.S. Geological Survey - Denver

Publication Type: Journal

Cui, T. J. & Chew, W. C. (1999, Jun.). Fast algorithm for electromagnetic scattering by buried conducting plates of large size. IEEE Trans. on Antennas and Propagation. 47(6), 1116-1118.

Cui, T. J. & Chew, W. C. (1999, Mar.). Fast evaluation of sommerfeld integrals for EM scattering and radiation by three-dimensional buried objects. IEEE Trans. on Geoscience and Remote Sensing, GE-37(2), 887-900.

Cui, T. J. & Chew, W. C. (1999, Sept.). Fast algorithm for electromagnetic scattering by buried 3D dielectric objects of large size. IEEE Trans. on Geoscience and Remote Sensing. GE-37(5), 2597-2608.

Cui, T. J. & Chew, W. C. (2000, Apr.). Accurate model of arbitrary wire antennas above ground. IEEE T. Antenn. Propag. 48(4), 482-493.

Cui, T. J. & Chew, W. C. (2000, Jan.). Modeling of arbitrary wire antennas above ground. IEEE T. Geosci. Remote. 38(1), 357-365, Part 2.

Publication Type: Paper

Cui, T. J. & Chew, W. C. (1999, Aug. 15-22). Fast algorithm for electromagnetic scattering by buried 3D dielectric objects of large size. XXVIth General Assembly of the International Union of Radio Science, 982. Toronto, Canada.

Cui, T. J. & Chew, W. C. (1999, Jul. 12-15). Accurate model of arbitrary wire antennas in free space, above or inside ground. Digest of IEEE Antennas and Propagation Society International Symposium. 2, 982-985. Orlando, FL.

Wright, D. L. et. al. (1999, Aug. 13-21). An assessment of the prototype very early time electromagnetic system (VETEM). XXVIth General Assembly of the International Union of Radio science. Toronto, Canada.

Wright, D. L., et. al. (1999, Mar. 14-18). New field and modeling results from a simulated waste pit using the enhanced very early time electromagnetic (VETEM) prototype system. Proceeding of the 12th Annual Symposium on the Applications of Geophysics to Environmental and Engineering Problem (SAGEEP). Oakland, CA.

Publication Type: Report

Cui, T. J. & Chew, W. C. (1999, Aug.). Novel difraction tomographic algorithm for imaging two-dimensional dielectric objects buried under a lossy

earth. Research Report, Electromagnetics Laboratory, University of Illinois at Urbana-Champaign. No. CCEM-21-99. Also submitted to IEEE Trans. on Geoscience and Remote Sensing.

Cui, T. J. & Chew, W. C. (1999, Jan.). Accurate model of arbitrary wire antennas in free space, above or inside ground. Electromagnetics Laboratory, University of Illinois at Urbana-Champaign, Research Report No. CCEM-2-99. Also submitted to IEEE Trans. on Antennas and Propagation.

Cui, T. J. & Chew, W. C. (1999, Jul.). Frequency-spatial domain inverse scattering of two-dimensional dielectric objects buried under a lossy earth. Research Report, Electromagnetics Laboratory, University of Illinois at Urbana-Champaign. No. CCEM-19-99. Also submitted to IEEE Trans. on Microwave Theory and Techniques.

Cui, T. J., et. al. (1999, Mar.). Numerical modeling of an enhanced very early time electromagnetic (VETEM) prototype system. Research Report, Electromagnetics Laboratory, University of Illinois at Urbana-Champaign. No. CCEM-7-99. Also submitted to IEEE Antennas and Propagation Magazine.

Cui, T. J., et. al. (1999, May). Nonlinear inverse scattering of two-dimensional dielectric objects buried under a lossy earth. Research Report, Electromagnetics Laboratory, University of Illinois at Urbana-Champaign. No. CCEM-12-99. Also submitted to IEEE Trans. on Geoscience and Remote Sensing.

Project: 60328

Title: High Frequency Electromagnetic Impedance Measurements for Characterization, Monitoring and Verification Efforts

PI: Dr. Ki-Ha Lee *Institution:* Lawrence Berkeley National Laboratory

Publication Type: Presentation

Lee, K. H., Becker, A., & Frangos, W. (2000, Apr.). High frequency impedance measurements for characterization, monitoring, and verification efforts. 2nd EMSP National Workshop. Atlanta, GA..

Lee, K. H., Becker, A., Pellerin, L., & Frangos, W. (1998, Jul.). High frequency impedance measurements for characterization, monitoring, and verification efforts. 1st EMSP National Workshop. Chicago, IL.

Song, Y., Morrison, H. F., & Lee, K. H. (1997). High frequency electromagnetic impedance for subsurface imaging. Symposium for Application of Geophysics to Engineering and Environmental Problems (SAGEEP). Reno, NV.

Publication Type: Report

Frangos, W. & Becker, A. (1998). Magnetic fields of AM band radio broadcast signals at the Richmond Field Station. Lawrence Berkeley National Lab Report LBNL-42654.

Project: 70108 (Renewal of Project No. 55411)

Title: Effects of Fluid Distribution on Measured Geophysical Properties for Partially Saturated, Shallow Subsurface Conditions

PI: Dr. Patricia A. Berge *Institution:* Lawrence Livermore National Laboratory

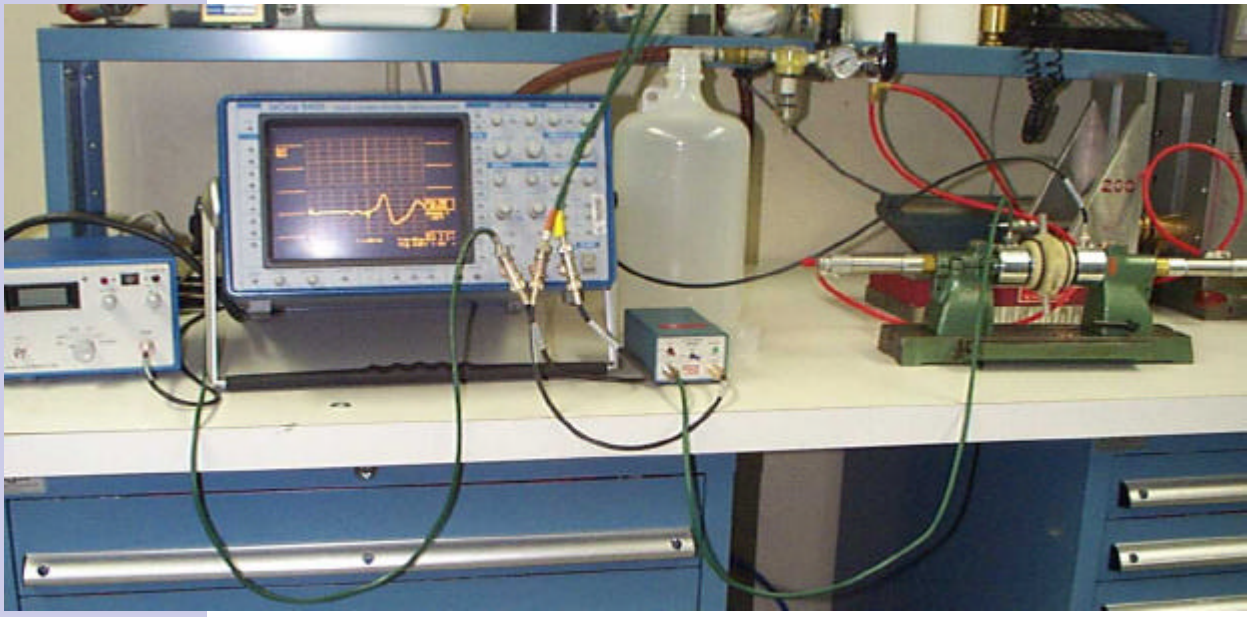
Publication Type: Journal

Berryman, J. G. & Pride, S. R. (1998). Volume averaging, effective stress rules, and inversion for microstructural response of multicomponent porous media. LLNL report UCRL-JC-127248, Int. J. Sol. Struct. 35, 4811-4843.

Berryman, J. G., Berge, P. A., & Bonner, B. P. (2000). Transformation of seismic velocity data to extract porosity and saturation values for rocks: LLNL Report UCRL-JC-136703. Journal of the Acoustical Society of America. 107, 3018-3027.

Berryman, J. G., Berge, P. A., & Bonner, B. P. (2001, in press). Estimating rock porosity and fluid saturation using only seismic velocities: LLNL report UCRL-JC-135507. Geophysics.

Pride, S. R. & Berryman, J. G. (1998). Connecting theory to experiment in poroelasticity. J. Mech. Phys. Sol. 46, 719-747.



Photograph of experimental apparatus for measuring ultrasonic compressional and shear wave velocities in soils at low pressures. The oscilloscope screen displays an amplified signal from the pulse generator at the far left. This signal travelled through the soil sample in the sample holder assembly to the right. [see Project #70108, renewal of #55411]

Wildenschild, D., Roberts, J. J., & Carlberg, E. D. (2000, in press). On the relationship between microstructure and electrical and hydraulic properties of sand-clay mixtures: LLNL Report UCRL-ID-136122. Geophysical Research Letters.

Wildenschild, D., Roberts, J. J., & Carlberg, E. D. (2000). On the relationship between microstructure and electrical and hydraulic properties of sand-clay mixtures: LLNL report UCRL-ID-136122. Geophysical Research Letters. 27,3085-3088.

Publication Type: Paper

Berryman, J. G. & Berge, P. A. (1999, Mar. 24-27). Mixture theory for predicting geomechanical coefficients of heterogeneous reservoirs. Fifth Society for Industrial and Applied Mathematics (SIAM) Conference on Mathematical and Computational Issues in the Geosciences. San Antonio, TX. 110.

Publication Type: Patent

Berryman, J.G. (1999, Oct. 4). Robust discrimination of porosity and fluid saturation using seismic velocity analysis. DOE Patent Docket No. S-92015, LLNL Patent disclosure IL-10437.

Bonner, B. P., Boro, C., & Hart, D. J. (1999, Oct. 28). Anti-waveguide for ultrasonic testing of granular media under elevated stress. DOE Patent Docket No. S-94182, LLNL Patent disclosure IL-10607.

Publication Type: Presentation

Roberts, J. J. (2000, Apr.). Preliminary results of the effects of fluid distribution on measured geophysical properties for partially saturated, shallow subsurface conditions. Environmental Management Science Program National Workshop, Atlanta, GA.

Roberts, J. J. (2000, Jan. 19-20). Results of the joint inversion of geophysical data for site characterization and restoration monitoring. Advanced Vadose Zone Characterization Workshop, Richland, WA.

Roberts, J. J. (2000, Jan.). Preliminary results of the effects of fluid distribution on measured geophysical properties for partially saturated, shallow subsurface conditions. Advanced Vadose Zone Characterization Workshop, Richland, WA.

Publication Type: Proceeding

Berge, P. A., Bonner, B. P., Aracne-Ruddle, C., Trombino, C., & Berryman, J. G. (1999). Compressional and shear wave velocities of soils at low pressures— Theoretical estimates, and comparison of laboratory and field data. LLNL report UCRL-JC-133211 Abs, Proceedings of the Seismological Society of America (SSA) 94th Annual Meeting, Seismological Research Letters. 70, 226.

Bonner, B. P., et. al. (1999, Mar. 14-18). Ultrasonic characterization of synthetic soils for application to near surface geophysics. Powers, M. H., Cramer, L., & Bell, R. S. (Eds.), Proceedings of the Symposium on the Application of Geophysics to Engineering and Environmental Problems (SAGEEP). Oakland, CA. Environmental and Engineering Geophysical Society. Wheat Ridge, CO. 455-463.

Bonner, B. P., et. al. (2001, in press). Linear and nonlinear ultrasonic properties of granular soils: LLNL report UCRL-JC-136207. Materials Research Society Spring Meeting, April 24-28, 2000. San Francisco, CA.

Bonner, B. P., Wildenschild, D., Berge, P. A., Ruddle, D., & Aracne-Ruddle, C. M. (2000). Ultrasonic velocities of artificial sediments with minimal overburden (abstract): LLNL report UCRL-JC-140230-ABS. Eos, Transactions of the American Geophysical Union, Fall Meeting Supplement. Proceedings of the Fall Annual Meeting, held in San Francisco, CA. Dec. 15-19, 2000. 81, F1105.

Publication Type: Report

Aracne-Ruddle, C. M., et. al. (1999). Ultrasonic velocities in unconsolidated sand/clay mixtures at low pressures: LLNL Report UCRL-JC-135621. Lawrence Livermore National Laboratory. Livermore, CA. Abs, Eos, Transactions of the American Geophysical Union, 80, Fall Meeting Supplement, F397.

Aracne-Ruddle, C., Wildenschild, D., Bonner, B., & Berge, P. (1998). Direct observation of morphology of sand-clay mixtures with implications for mechanical properties in sediments. LLNL report UCRL-JC-131702 Abs, Eos, Transactions of the American Geophysical Union, 79, Fall Meeting Supplement, F820.

Aracne-Ruddle, C., Wildenschild, D., Bonner, B., & Berge, P. (1998, Oct. 15-16). Direct observation of fluid-clay interactions with implications for mechanical and electrical properties. LLNL report UCRL-JC-131116 Abs. Presentation at the LLNL Women's Technical and Professional Symposium. San Ramon, CA.

Berge, P. A. & Berryman, J. G. (1999, Mar. 24-27). Developing rock physics algorithms for velocity-porosity relations with environmental geophysics applications. LLNL report UCRL-JC-132054 Abs, Fifth Society for Industrial and Applied Mathematics (SIAM) Conference on Mathematical and Computational Issues in the Geosciences. San Antonio, TX. 108.

Berge, P. A. & Bertete-Aguirre, H. (2000, Feb. 20-24). Laboratory velocity measurements used for inferring soil distributions from field seismic data: LLNL Report UCRL-JC-135132. In Powers, M. H., Ibrahim, A. -B., & Cramer, L. (Eds.). Proceedings of the 13th Annual Symposium on the Application of Geophysics to Engineering and Environmental Problems (SAGEEP). Arlington, VA. Environmental and Engineering Geophysical Society. Wheat Ridge, CO. 185-194.

Berge, P. A. (2000). Final report for EMSP project 55411, Joint inversion of geophysical data for site characterization and restoration monitoring: LLNL report UCRL-ID-128343. Lawrence Livermore National Laboratory. Livermore, CA.

Berge, P. A. (2000). FY2000 annual report for EMSP project 70108, Effects of fluid distribution on measured geophysical properties for partially saturated, shallow subsurface conditions: LLNL report UCRL-ID-137130. Lawrence Livermore National Laboratory. Livermore, CA.

Berge, P. A. (2000). Powerpoint presentation on effects of fluid distribution on measured geophysical properties for partially saturated, shallow subsurface conditions: LLNL report UCRL-VG-137423 rev. 1. Advanced Vadose Zone Characterization Workshop. PNNL Hanford Groundwater/Vadose Zone Integration Project, held Jan. 19-20, 2000. Richland, WA.

Berge, P. A. (2000). Powerpoint presentation on EMSP project 70108: Effects of fluid distribution on measured geophysical properties for partially saturated, shallow subsurface conditions: LLNL report UCRL-VG-137423. EMSP Principal Investigator Orientation Meeting, held Nov. 16-18, 1999. Richland, WA.

Berge, P. A. (2000, Apr. 25-27). EMSP project 70108: Effects of fluid distribution on measured geophysical properties for partially saturated, shallow subsurface conditions: LLNL report UCRL-JC-137130-ABS rev. 1. Science Advancing Solutions EMSP National Workshop Guidebook for the Environmental Management Science Program (EMSP) National Workshop.

Berge, P. A., Berryman, J. G., Bonner, B. P., Roberts, J. J., & Wildenschild, D. (1998, Oct. 15-16). Preliminary results from an environmental geophysics project for improving geophysical imaging of fluid distribution in the shallow subsurface. LLNL report UCRL-JC-131209 Abs. Presentation at the LLNL Women's Technical and Professional Symposium. San Ramon, CA.

Berge, P. A., Berryman, J. G., Bonner, B. P., Roberts, J. J., & Wildenschild, D. (1999, Mar. 14-18). Comparing geophysical measurements to theoretical estimates for soil mixtures at low pressures. LLNL report UCRL-JC-132893. Powers, M. H., Cramer, L., & Bell, R. S. (Eds.), Proceedings of the Symposium on the Application of Geophysics to Engineering and Environmental Problems (SAGEEP), Oakland, CA. Environmental and Engineering Geophysical Society. Wheat Ridge, CO. 465-472.

Berge, P. A., Berryman, J. G., Roberts, J. J., & Wildenschild, D. (1998, Jul. 27-30). Joint inversion of geophysical data for site characterization and restoration monitoring. EMSP project summary/progress report for FY98 for EMSP project 55411. LLNL report UCRL-JC-128343, presented at the DOE Environmental Management Science Workshop, Chicago, IL.

Berge, P. A., Berryman, J. G., Roberts, J. J., & Wildenschild, D. (1997). Joint inversion of geophysical data for site characterization and restoration monitoring. Carrigan, C. R. & Jackson, K. J. (Eds.), Environmental Management Science Program: Fiscal Year 1997 Progress Report, Lawrence Livermore National Laboratory (LLNL) report UCRL-ID-129562, LLNL, Livermore, CA.

Berryman, J. G., Berge, P. A., & Bonner, B. P. (1999, Oct. 31-Nov. 5). Role of lambda diagrams in estimating porosity and saturation from seismic velocities (expanded abstract): LLNL Report UCRL-JC-134224. Society of Exploration Geophysicists International Exposition and 69th Annual Meeting Technical Program. Houston, TX. Vol. I, 176-179.

Berryman, J., Dvorkin, J., Le Ravalec, M., & Nur, A. (1997). Effective moduli of particulates with elastic cement. LLNL report UCRL-JC-128340.

Bertete-Aguirre, H. & Berge, P. A. (1999). Laboratory ultrasonic measurements of sand-clay mixtures used to recover clay content in silty sands (abstract): LLNL Report UCRL-JC-135643. Abs, Eos, and Transactions of the American Geophysical Union, 80, Fall Meeting Supplement. F395-396.

Bonner, B. P., Hart, D. J., Berge, P. A., & Aracne, C. M. (1997). Influence of chemistry on physical properties: Ultrasonic velocities in mixtures of sand and swelling clay. LLNL report UCRL-JC-128306abs, Eos, Transactions of the American Geophysical Union, 78, Fall Meeting Supplement, F679.

Rowe, C. D. (1997, summer). Joint inversion of geophysical data for site characterization and restoration monitoring. In Williams, B. (Ed.), The Associated Western Universities Summer Participant Program at the Lawrence Livermore National Laboratory, Summer 1997: LLNL report UCRL-ID-128721-97, LLNL. Livermore, CA. 75-78.

Trombino, C. N. (1998). Elastic properties of sand-peat moss mixtures from ultrasonic measurements. LLNL report UCRL-JC-131770. LLNL, Livermore, CA.

Wildenschild, D., Roberts, J. J. & Carlberg, E. D. (1998). Transport and microstructural properties of sand-clay mixtures. LLNL report UCRL-JC-131703 Abs, Eos, Transactions of the American Geophysical Union, 79, Fall Meeting Supplement, F820.

Wildenschild, D., Roberts, J. J., & Carlberg, E. (1999, Mar. 14-18). Influence of microstructural properties on geophysical measurements in sand-clay mixtures. LLNL report UCRL-JC-131557. Powers, M. H., Cramer, L., & Bell, R.S. (Eds.), Proceedings of the Symposium on the Application of Geophysics to Engineering and Environmental Problems (SAGEEP). Oakland, CA. Environmental and Engineering Geophysical Society. Wheat Ridge, CO. 445-454.

Wildenschild, D., Roberts, J. J., & Carlberg, E. D. (1999, Oct. 31-Nov. 5). Electrical properties of sand-clay mixtures: The effect of microstructure (expanded abstract): LLNL Report UCRL-JC-135208. Society of Exploration Geophysicists International Exposition and 69th Annual Meeting Technical Program. Houston, TX. Vol. I, 461-464.

Project: 73731 (Renewal of Project No. 60199)

Title: Automating Shallow Seismic Imaging

PI: Dr. Don W. Steeples *Institution:* University of Kansas

Publication Type: Journal

Baker, G. S., Schmeissner, C., Steeples, D. W., & Plumb, R. G. (1999). Seismic reflections from depths of less than two meters. Geophys. Res. Lett. 26(2), 279-282.

Baker, G. S., Steeples, D. W., & Schmeissner, C. (1999). In-situ, high-frequency P-Wave velocity measurements within 1 m of the Earth's surface. Geophysics. 64(2), 323-325.

(a) (b)

Field Layout. (a) View from one end of the plow. The channel iron with geophones and wiring attached runs from lower right to just above center of photo. (b) Plow with test-line geophones planted in the ground under the rear of the plow. Comparison-line geophones with normal plants are about 75cm to the right of the test line. [see Project #73731, renewal of #60199]

(a)

(b)

Automatic geophone-planting device. (a) Folded plow, ready for transport. Channel iron welded to V-shaped blades can be seen at top right. (b) Plow ready for automatic geophone planting. Channel iron with geophones attached can be seen in the foreground as a white line running from left to right. [see Project #73731, renewal of #60199]

Baker, G. S., Steeples, D. W., Schmeissner, C., & Spikes, K. T. (2000, Apr.). Source-dependent frequency content of ultrashallow seismic reflection data. B. Seismol. Soc. Am. 90(2), 494-499.

Baker, G. S., Steeples, D. W., Schmeissner, C., & Spikes, K. T. (2000). Ultrashallow seismic reflection monitoring of seasonal fluctuations in the water table. Environ. Engrg. Geosci. 6, 271-277.

Baker, G. S., Steeples, D. W., Schmeissner, C., & Pavlovic, M. (2000, in press). On coincident seismic and radar imaging. Geophysics.

Baker, G. S., Steeples, D. W., Schmeissner, C., Pavlovic, M., & Plumb, R. (2001). Coincident imaging using seismic and GPR data. Geophys. Res. Lett. 28(4), 627-630.

Steeples, D. W. & Baker, G. S. (1998, Jun.). Near-surface contributions to seismic static corrections. AAPG Explorer. 19, 20-21, 29.

Steeples, D. W., Baker, G. S., & Schmeissner, C. (1999). Toward the autojuggie: Planting 72 geophones in 2 seconds, Geophysical Research Letters. 26(8), 1085-1088.

Steeples, D. W., Baker, G. S., Schmeissner, C., & Macy, B. K. (1999). Geophones on a board. Geophysics. 64(3), 809-814.

Publication Type: Poster

Plumb, R. G., Steeples, D. W., Baker, G. W., Schmeissner, C., & Pavlovic, M. (1999, Jun.). A combined ground-penetrating radar and shallow seismic reflection approach to characterizing hydrological flow. International Geoscience and Remote Sensing Society (IGARSS) meeting. Hamburg, Germany.

Publication Type: Presentation

Baker, G. S., Plumb, R. G., Steeples, D. W., Pavlovic, M., & Schmeissner, C. (1998). Coincident GPR and ultrashallow seismic imaging in the Arkansas River Valley, Great Bend, Kansas. SEG Expanded Abstracts, SEG 1998 International Meeting. New Orleans, LA. 859-861.

Baker, G. S., Steeples, D. W., Schmeissner, C., & Macy, B. K. (1998). In-situ, high-resolution P-wave velocity measurements within 1 m of the Earth's surface. SEG Exp. Abstr., SEG 1998 International Meeting. New Orleans, LA. 856-858.

Steeples, D. W., Baker, G. S., & Schmeissner, C. (1998, Dec. 6-10). Toward the autojuggie: Planting 72 geophones in 2 seconds. (1998). American Geophysical Union, 1998 Fall Meeting. San Francisco, CA.

Steeples, D. W., Baker, G. S., Schmeissner, C., & Macy, B. K. (1998). Geophones on a board. SEG Exp. Abstr., SEG 1998 International Meeting. New Orleans, LA. 852-855.

Publication Type: Proceeding

Baker, G. S., McIntyre, C., Walczak, L., & Steeples, D. W. (2000, Aug. 6-11). Improving ultrashallow seismic reflection data by reducing source energy. Exp. Abstr. SEG Intl. Exposition and 70th Annual Meeting. Calgary, Alberta, Canada. II, 1267-1270.

Baker, G. S., Steeples, D. W., Schmeissner, C., & Spikes, K. T. (2000). Collecting seismic-reflection data from depths shallower than three meters. Proceeding of the Symposium on the Application of Geophysics to Engineering and Environmental Problems (SAGEEP). Washington, D. C. 1207-1214.

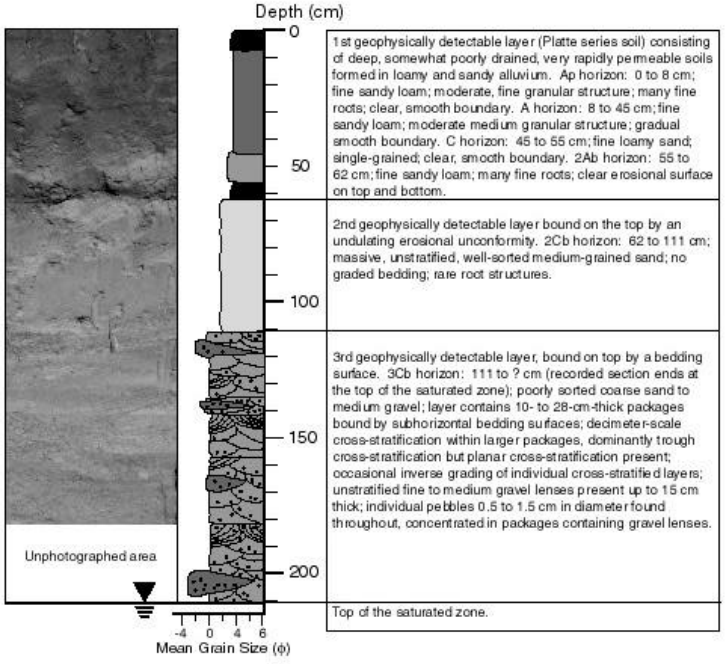
Schmeissner, C., Steeples, D. W., Pavlovic, M., Prado, R., & Spikes, K. T. (2000, Aug. 6-11). Recording seismic reflections using rigidly imterconnected geophones. Exp. Abstr. SEG Intl. Exposition and 70th Annual Meeting. Calgary, Alberta, Canada. II, 1279-1282.

Spikes, K. T., Steeples, D. W., Schmeissner, C., & Prado, R. (2000, Aug. 6-11). Varying the effective mass of geophones. Exp. Abstr. SEG Intl. Exposition and 70th Annual Meeting. Calgary, Alberta, Canada. II.

Steeples, D. W., Schmeissner, C. M., & Baker, G. S. (2000, Apr. 10-12). Applications of and recent developments in shallow seismic reflection. Abstract, SSA 95th Annual Meeting. San Diego, CA. Seismological Research Letters. 71(2), 231.

Publication Type: Theses/Dissertations

Baker, G. S. (1999, May). Seismic imaging shallower than three meters. Ph. D. dissertation. The University of Kansas. Lawrence, KS.



Photograph, stratigraphic column, and description of hand-dug hole located approximately 15m from seismic and GPR lines. Ground-penetrating radar successfully imaged the two upper interfaces but not the top of the saturated zone. The seismic-reflection technique imaged the three main interfaces. Both techniques imaged some reflectors within the main layers, interpreted as cross-bedding or unidentified lenses. [see Project #73731, renewal of #60199]

Pavlovic, M. (2000). Ground-penetrating radar in shallow aquifer detection and monitoring. Master's Thesis. University of Kansas. Lawrence, KS.

Project: 73776 (Renewal of Project No. 60328)

Title: High Frequency Electromagnetic Impedance Measurements for Characterization, Monitoring and Verification Efforts

PI: Dr. Ki-Ha Lee *Institution:* Lawrence Berkeley National Laboratory

Publication Type: Patent

Becker, A. (1998, Jan. 8). High-frequency electric field measurement using a toroidal antenna. Provisional Application Ser. No. 60/070,850.

Publication Type: Presentation

Lee, K. H., Becker, A., Pellerin, L., & Frangos, W. (1998, Jul.). High frequency impedance measurements for characterization, monitoring, and verification efforts. 1st EMSP National Workshop. Chicago, IL.

Lee, K. H., Becker, A., Pellerin, L., & Frangos, W. (2000, Apr.). High frequency impedance measurements for characterization, monitoring, and verification efforts. 2nd EMSP National Workshop. Atlanta, GA.

Song, Y., Morrison, H. F., & Lee, K. H. (1997). High frequency electromagnetic impedance for subsurface imaging. Symposium for Application of Geophysics to Engineering and Environmental Problems (SAGEEP). Reno, NV.

Publication Type: Report

Frangos, W. & Becker, A. (1998). Magnetic fields of AM band radio broadcast signals at the Richmond Field Station. Lawrence Berkeley National Lab Report LBNL-42654.

Lee, K. H. (1997). High-frequency electric field measurement using a toroidal antenna. Lawrence Berkeley National Lab Report LBNL-39894, UC-2040.

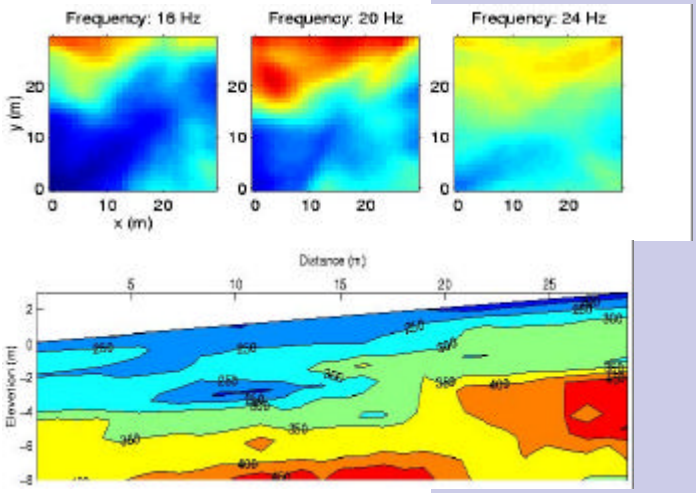
Project: 73830 (Renewal of Project No. 55218)

Title: Seismic Surface-Wave Tomography of Waste Sites

PI: Dr. Timothy L. Long *Institution:* Georgia Institute of Technology

Publication Type: Journal

Long, L. T. & Kocaoglu, A. (2001, in press) Surface-wave group-velocity tomography for shallow structures. Journal of Environmental and Engineering Geophysics.



Ever wonder what is under here? Generate a set of Group Velocity images (upper right), then invert the dispersion curves at each position to get an image of the shear-wave structure (lower right). The low velocity at 10m and 4m depth is a suspected burial trench, or the high uplifted under 25m could indicate a thrust fault. [see Project #73830, renewal of #55218]

Publication Type: Other

Long, L. T. (1999, Feb.). Seismic surface wave tomography at waste sites. Research Note in Fast Times, the EEGS Newsletter.

Publication Type: Presentation

Long, L. T. & Kocaoglu, A. (1999, Oct. 16-20). A tomographic inversion method for near-surface structure. Eastern Section Seismological Society of America Annual Meeting. Memphis, TN.

Long, L. T., Kocaoglu, A., Doll, W. E., Chen, X. Q., & Martin, J. (1999, Oct.). Surface-wave group-velocity tomography for shallow structures at a waste site. SEG Expanded Abstract, Annual Meeting. Houston, TX.

Publication Type: Proceeding

Long, L. T., & Kocaoglu, A. (1999, Mar.). Surface-wave group-velocity tomography for shallow structures. Proceedings of the Symposium on the Application of Geophysics to Engineering and Environmental Problems, Environmental and Engineering Geophysical Society (SAGEEP99).

Martin, J., Long, L. T., & Kubota, T. (2000, Sept. 10-13). Imaging near-surface buried structure with high-resolution surface-wave group-velocity tomography. Proceedings of the IEEE Signal Processing Society, International Conference on Image Processing. Vancouver, British Columbia, Canada.

Project: 73962 (Renewal of Project No. 60115)

Title: Advanced High Resolution Seismic Imaging, Material Properties Estimation and Full Wavefield Inversion for the Shallow Subsurface

PI: Dr. Alan R. Levander *Institution:* Rice University

Publication Type: Journal

Zelt, C. A., Hojka, A. M., Flueh, E. R., & McIntosh, K. D. (1999, Aug. 15). 3D simultaneous seismic refraction and reflection tomography of wide-angle data from the central Chilean margin. Geophys. Res. Lett. 26(16), 2577-2580.

Zelt, C. A., Optimal utilization of sub-optimal 3D wide-angle data. Seis. Res. Lett. 70, 255.

Publication Type: Presentation

Akerberg, P., Dana, D., Levander, A., Zelt, C., & Henstock, T. (1998). High resolution shallow seismic imaging at an open pit copper mine. 10th Annual IRIS Workshop. Santa Cruz, CA.

Dana, D., Akerberg, P., Levander, A., Zelt, C., & Henstock, T. J. (1998). Shallow-seismic investigation at an open pit copper mine: A comparison with drill data. EOS, Trans. Am. Geophys. Union. 79, F652.

Dana, D., Akerberg, P., Zelt, C., Levander, A., & Henstock, T. (1998). High resolution seismic imaging at a porphyry copper mine. Society of Exploration Geophysicists. New Orleans, LA.

Dana, D., Zelt, C., & Levander, A. (1999). High-resolution seismic survey over a near-surface contamination site. SEG International Exposition and Sixty-Ninth Annual Meeting.

Passmore, P., Keller, G. R., Miller, K. C., Levander, A., & McMechan, G. (1999). Single-channel recorder test results from two different active source experiments. Seism. Res. Letters. 70, 243.

Zelt, C. A. & Hojka, A. M. (1998). 3D simultaneous seismic refraction and reflection tomography of wide-angle traveltime data from the central Chilean margin. EOS. 79, F638.

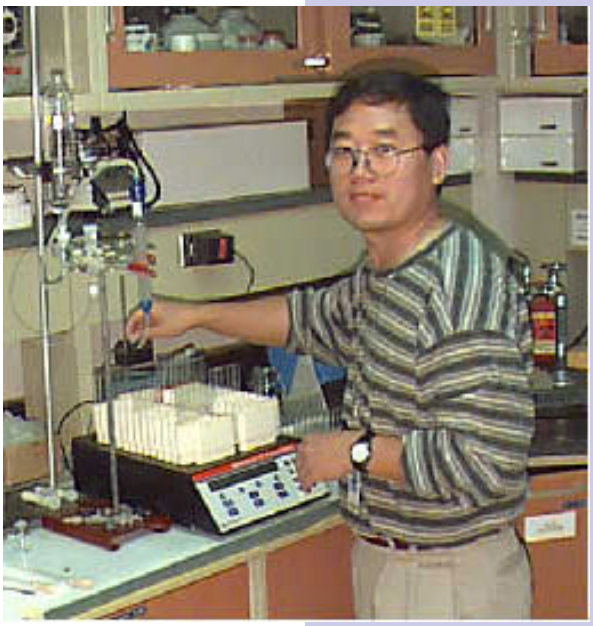
Health/Risk

Project: 55033

Title: Characterization of Chemically Modified Hyperthermophilic Enzymes for Chemical Syntheses and Bioremediation Reactions

PI: Dr. Brian H. Davison *Institution:* Oak Ridge National Laboratory

Publication Type: Journal



Purification of the PEG-modified enzymes using gel permeation chromatography. [see Project #55033]

Kim, C., Brereton, P. S., Verhagen, M. F. J. M., & Adams, M. W. W. (2000, in press). Ferredoxin from Pyrococcus furiosus. Meths. Enzymol.

Kim., C., Woodward, C. A., Kaufman, E. N., & Adams, M. W. W. (1999). Stability and sulfur reduction activity in organic media of hydrogenase from the hyperthermophilic Pyrococcus furiousus. Biotechnologies & Bioengineering. 65, 108-113.

Ma, K. & Adams, M. W. W. (2000, in press). Hydrogenase I and hydrogenase II from Pyrococcus furiosus. Meths. Enzymol.

Ma, K., Weiss, R., & Adams, M. W. W. (2000). Characterization of hydrogenase II from the hyperthermophilic archaeon Pyrococcus furiosus and assessment of its role in sulfur reduction. J. Bacteriol. 182, 1864-1871.

Sapra, R., Verhagen, M. F. J. M., & Adams, M. W. W. (2000). Purification and characterization of a membrane-bound hydrogenase from the hyperthermophilic archaeon Pyrococcus furiosus. J. Bacteriol. 182, 3423-3428.

Telser, J., Davydov, R., Kim, C-H., Adams, M. W. W., & Hoffman, B. M. (1999). Investigation of the unusual electronic structure of Pyrococcus furiosis 4Fe ferredoxin by EPR spectroscopy of protein reduced at ambient and cryogenic temperatures. Inorganic Chemistry. 38, 3550-3553.

Wang, P., Woodward, C. A., & Kaufman, E. N. (1999). Poly(ethylene glycol)-modified ligninase enhances pentachlorophenol biodegradation in water-solvent mixtures. Biotechnologies & Bioengineering. 64, 290-297.

Publication Type: Poster

Adams, M. W. W. (1995). Properties of polyethylene glycol-modified proteins in aqueous and organic media. Inorganic Biochemistry Summer Workshop ’95. Athens, GA.

Adams, M. W. W. (1996). Polyethylene glycol-modified hydrogenase from pyrococcus furiosis that is soluble and active in organic solvents. Thermophiles ’96: International Conference on the Biology, Ecology, and Biotechnology of Thermophilic Microorganisms. Athens, GA.

Wang, P., et. al. (1998, May). PEG-modified ligninase enhances pentachlorophenol biodegradation in water-solvent mixtures. NSF Thermophile Workshop. Seattle, WA.

Publication Type: Presentation

Adams, M. W. W. (1996). Enzymatic catalysis in organic solvents: Polyethylene glycol modified hydrogenase is soluble in toluene and retains sulfur-reducing activity. The 18th Symposium on Biotechnology for Fuels and Chemicals. Gatlingburg, TN.

Adams, M. W. W. (1998, Jul.). Characterization of chemically modified enzymes for bioremediation reactions. EMSP Review Meeting. Chicago, IL.

Adams, M. W. W. (2000, Apr.). Characterization of chemically modified enzymes for bioremediation reactions. EMSP Review Meeting. Atlanta, GA.

Davison, B. (1998, May). A new phase for nonaqueous biocatalysis. Oak Ridge National Laboratory Showcase Seminar.

Kaufman, E., et. al. (1996, Nov.). Enzymatic catalysis in organic solvent: Polyethylene glycol modified hydrogenase retains sulfohydrogenase activity in tolunene. AIChE Annual Meeting.

Wang, P., et. al. (1998, May). Modification of enzymes for non-aqueous catalysis: Bioremediation of chlorinated pollutants in organic solvents. 1st Annual Conference on the Remediation of Chlorinated and Recalcitrant Compounds. Columbus, OH.

Wang, P., et. al. (1998, Nov.). Activation and stabilization of ligninase for remediation of polychlorinated pollutants in organic solvents. AIChE Annual Meeting. Miami Beach, FL.

Publication Type: Proceeding

Adams, M. W. W. (1996). Hyperthermophilic proteins from Pyrococcus furiosis that are soluble and active in a pure organic solvent. The 3rd Annual National Science Foundation Hyperthermophile Symposium. Raleigh, NC.

Adams, M. W. W. (1997). Enzymatic catalysis in organic solvents. The 4th Annual National Science Foundation Hyperthermophile Symposium. Del Mar, CA.

Adams, M. W. W. (1998). Catalytic and spectroscopic studies of polyethylene glycol-modified, hyperthermophilic proteins in organic solvents. The 5th Annual National Science Foundation Hyperthermophile Symposium. Seattle, WA.

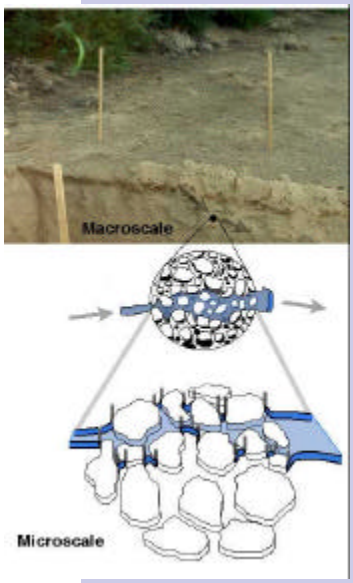
Adams, M. W. W. (1999). Properties of the ferredoxin iron-sulfur cluster from the hyperthermophilic archaeon Pyrococcus furiosis in organic solvents. The 6th Annual National Science Foundation Hyperthermophile Symposium. Athens, GA.

Hydrogeology

Project: 54576

Title: On the Inclusion of the Interfacial Area Between Phases in the Physical and Mathematical Description of Subsurface Multiphase Flow

PI: Dr. William G. Gray *Institution:* University of Notre Dame



The specific effects of interfacial behavior between interfaces that separate different fluids or separate fluids from solids is being more carefully studied so that their net impacts on fluid flow the macroscopic scale can be better understood. [see Project #54576]

Publication Type: Journal

Gray, W. G. & Miller, C. T. (2000, Feb.). Comment on 'Dynamics of wetting fronts in porous media' by Mitkov, I., Tartakovsky, D. M., & Winter, C. L. Physical Review E. 61(2), 2150-2151.

Gray, W. G. (2000, Mar.). Macroscale equilibrium conditions for two-phase flow in porous media. Int. J. Multiphas. Flow. 26(3), 467-501.

Hazlett, R. D., Chen, S. Y., & Soll, W. E. (1998, Jun.). Wettability and rate effects on immiscible displacement: Lattice Boltzmann Simulation in Microtomographic Images of Reservoir Rocks. J. of Petroleum Science and Engineering. 20(3-4), 167-175.

Hou, S., Shan, X., Zou, Q., Doolen, G. D., & Soll, W. E. (1997). Evaluation of two Lattice Boltzmann models for multiphase flow. J. of Computational Physics, 138. 695-713.

Soll, W. E., Gray, W. G., Janecky, D. R., & Thompson, A. F. B. (1997, Nov. 4). Meeting Report: Linking the pore and continuum scales through theory, modeling, and experimentation. EOS, Transactions, American Geophysical Union. 78(44), 495.

Publication Type: Other

Gray, W. G. (1999, Apr.). Elements of a systematic procedure for the derivation of macroscale conservation equations for multiphase flow in porous media. Hutter, K. & Wilmanski, K. (Eds.). Kinetic and Continuum Thermodynamical Approaches to Granular and Porous Media. CISM Courses and Lectures No. 400, International Centre for Mechanical Sciences. Springer-Verlag, Vienna, Austria. 67-129.

Hassanizadeh, S. M. & Gray, W. G. (1997, Oct.). Basic equations of flow and transport in porous media. Sikdar, S. K. & Irvine, R. L. (Eds.). Bioremediation: Principles and Practice, Vol. I, Fundamentals and Applications. Technomic Publishing Company, Inc. 19-57.

Soll, W. E., Gray, W. G. & Tompson, A. F. B. (1998). Influence of wettability on constitutive relations and its role in upscaling. V. N. Burganos, et. al. (Eds.), Computational Methods in Water Resources XII, Computational Mechanics Publications, Southampton. Vol. 1, 413-420

Publication Type: Paper

Gray, W. G. (1999, Jan.). Thermodynamics and constitutive theory for multiphase porous-media flow considering internal geometric constraints. Advances in Water Resources. 22(5), 521-547.

Gray, W. G., & Hassanizadeh, S. M. (1998, July). Macroscale continuum mechanics for multiphase porous-media flow including phases, interfaces, common lines, and common points. Advances in Water Resources. 21(4), 261-281.

Muccino, J. C., Gray, W. G., & Ferrand, L. A. (1998, Aug.). Toward an improved understanding of multiphase flow in porous media. Reviews of Geophysics. 36(3), 401-422.

Project: 54908

Title: Partitioning Tracers for In Situ Detection and Quantification of Dense Non-aqueous Phase Liquids in Groundwater Systems

PI: Dr. Mark L. Brusseau *Institution:* University of Arizona

Publication Type: Journal

Brusseau, M. L. (1992, Dec.). Factors influencing the transport and fate of contaminants in the subsurface. J. Hazard. Mater. 32(2-3), 137-143.

Brusseau, M. L., Nelson, N. T., & Costanza, M. S. (1999, in press). Partitioning tracer tests for characterizing immiscible-fluid saturations and interfacial areas in subsurface systems.

Nelson, N. T., et. al. (1999, Dec.). A gas-phase partitioning tracer method for the in situ measurement of soil-water content. Water Resour. Res. 35(12), 3699-3707.

Nelson, N. T., Oostrom, M., Wietsma, T. W., & Brusseau, M. L. (1999, Nov. 15). Partitioning tracer method for the in situ measurement of DNAPL saturation: Influence of heterogeneity and sampling method. Environ. Sci. Technol. 33(22), 4046-4053.

Project: 55036

Title: Colloid Transport and Retention in Fractured Deposits

PI: Dr. John F. McCarthy *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

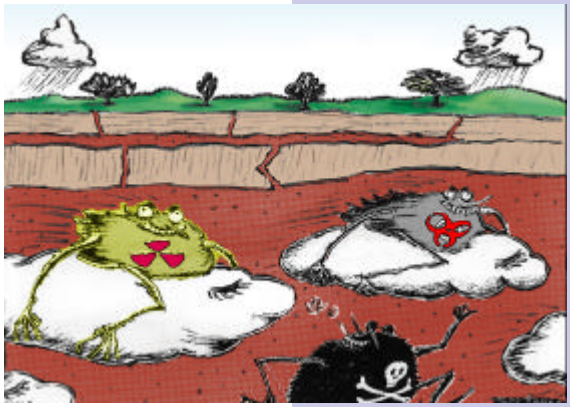
Cumbie, D. H. & McKay, L. D. (1999). Influence of diameter on particle transport in a fractured shale saprolite. J. Contam. Hydrol. 37, 139-157.

McCarthy, J. F. & Shevenell, L. (1998). Obtaining representative ground water samples in fractured and karst formations. Ground Water. 36(2), 251-260.

McCarthy, J. F. & Shevenell, L. (1998). Processes controlling colloid composition in a fractured and karstic aquifer in eastern Tennessee, USA. J. Hydrol. 206(3-4), 191-218.

McCarthy, J. F., Howard, K. M., & McKay, L. D. (1999, in press). Effect of pH on transport of flourobenzoic acid groundwater tracers. J. Contam. Hydrol.

McCarthy, J. F., Howard, K. M., & McKay, L. D. (2000, in press). Influence of pH on the behavior of fluorobenzoic acids as groundwater tracers. J. Environ. Qual.



Mobile colloids in the subsurface environment may alter the transport of contaminants. [see Project #55036]

Publication Type: Theses/Dissertations

Cumbie, D. H. (1997). Influence of diameter on particle transport in a fractured shale saprolite. Master's Thesis. University of Tennessee. Knoxville, TN.

Haun, D. D. (1998). The influence of ionic strength and cation valence on transport of colloi-size microspheres in fractured shale saprolite role of electrostatic attachment on particle transport in fractured shale saprolite. Masters thesis at the University of Tennessee.

Haun, D. D. B. (1998). Influence of ionic strength and cation valence on trasport of colloid-sized microspheres in fractured shale saprolite. Master's Thesis. University of Tennessee. Knoxville, TN.

Howard, K. H. (1997). Behavior of flourobenzoic acid groundwater tracers in a highly fractured shale saprolite. Masters thesis at the University of Tennessee.

Howard, K. H. (1998). Influence of pH on the behavior of fluorobenzoic acids as groundwater tracers. Master's Thesis. University of Tennessee. Knoxville, TN.

Oswald, J. (1999). Numerical modeling of colloid transport in discretely fractured porous media. PhD dissertation at Ohio State University.

Oswald, J. (projected 2000). Migration of colloids in discretely-fractured porous media: Effect of matrix diffusion. Ph. D. dissertation. Ohio State University. Columbus, OH.

Project: 55083

Title: Behavior of Dense, Immiscible Solvents in Fractured Clay-Rich Soils

PI: Dr. Larry D. McKay *Institution:* University of Tennessee at Knoxville

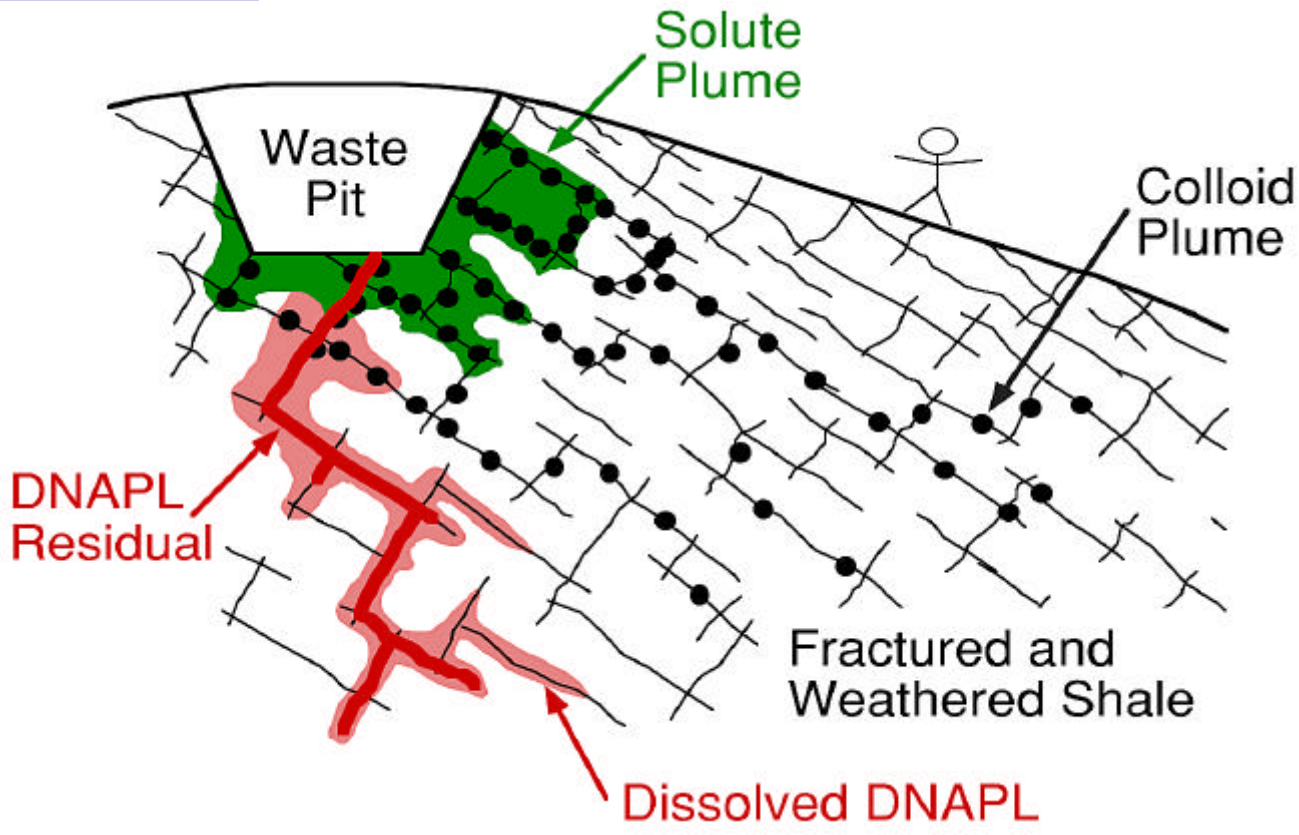
Publication Type: Journal

O'Hara, S. K., Parker, B. L., Jorgensen, P. R., & Cherry, J. A. (2000, Jan). Trichloroethene DNAPL flow and mass distribution in naturally fractured clay: Evidence of aperture variability. Water Resour. Res. 36(1), 135-147.

Publication Type: Presentation

Lenczewski, M., McKay, L. D., Sanseverino, J., & Knight, C. (1998, May 14-16). Sorption and microbiological factors controlling the fate and transport of TCE in fractured shale saprolite. Conference on Mass Transport in Fractured Aquifers and Aquitards, Univ. of Copenhagen, Denmark.

Lenczewski, M., McKay, L. D., Sanseverino, J., & Layton, A. (1999, May 30 - Jun. 3). Biodegradation of TCE in fractured weathered shale in east Tennessee. Annual Meeting of the American Society of Microbiology. Chicago, IL.



Migration of different contaminant types in fractured shales at Oak Ridge National Laboratory. Colloids migrate fastest, up to 200 m/day, because they are largely confined to fast-flow pathways in the fractures. Solutes, such as tritium, are strongly retarded relative to colloids because of diffusion into the relatively immobile pore water in the fine-grained matrix between fractures. DNAPLs can rapidly infiltrate downwards through the fractures, and then slowly dissolve forming plumes in the fractures and matrix pores. [see Project #55083]

Lenczewski, M., McKay, L. D., Sanseverino, J., & Layton, A. (1999, Apr. 12-14). Biodegradation of TCE in fractured shale saprolite. Annual Meeting of the Tennessee Water Resources Association. Nashville, TN.

McKay, L., et al., (1998, Jul. 27-30). Behavior of dense, immiscible solvents in fractured clay-rich soils. Poster presented at DOE/EMSP Workshop. Chicago, IL.

McKay, L.D. (1998, May 14-16). Contaminant transport in highly weathered and fractured shales. Conference on Mass Transport in Fractured Aquifers and Aquitards. Univ. of Copenhagen, Denmark.

McKay, L.D. (1999, May 11-13). Field and laboratory studies of DNAPL behavior in fractured and highly weathered shale. University Consortium Solvents-in-Groundwater Workshop, Queen's University. Kingston, Ontario, Canada.

O'Hara, S. (1999, May 11-13). Characterizing solvent DNAPL migration pathways in fractured clay using a large column laboratory experiment. University Consortium Solvents-in-Groundwater Workshop, Queen's University. Kingston, Ontario, Canada.

O'Hara, S. K., Parker, B. L., Slough, K. J., & Sudicky, E. A. (1998, Dec.). Characterizing solvent DNAPL migration pathways in fractured clay using a numerical model and a large column laboratory experiment. American Geophysical Union (AGU) Fall Meeting, San Francisco, CA.

Parker, B. L., O'Hara, S. K., & Kirkpatrick, G. A. (1998, May 18-21). Solvent DNAPL flow in naturally fractured clay: Laboratory and field experiments. Presented at the First International Conference on Remediation of Chlorinated and Recalcitrant Compounds. Monterey, CA.

Parker, B.L. (1998, May 14-16). Diffusion profiles for identifying DNAPL migration pathways in a glaciolacustrine fractured clay. Conference on Mass Transport in Fractured Aquifers and Aquitards. Univ. of Copenhagen, Denmark.

Pitner, A., McKay, L. D., & Lenczewski, M. (1999, Apr. 12-14). DNAPL entry, dissolution, and diffusion in fractured shale saprolite. Annual Meeting of the Tennessee Water Resources Association. Nashville, TN.

Publication Type: Theses/Dissertations

Cropper, S.C. (1998). Experimental observations of capillary pressure - saturation drainage of air and DNAPL in fractured shale saprolite. MS Thesis, Univ. of Tennessee. Knoxville, TN.

Lenczewski, M. E. (2000). Biodegradation of TCE in fractured shale and saprolite. Ph. D. Dissertation. University of Tennessee. Knoxville, TN.

O'Hara, S. K. (1997). Solvent DNAPL flow and matrix diffusion in natural fractured clay: A large column experiment. MS thesis, Univ. of Waterloo. Ontario, Canada.

Pitner, A. H. (2000). Experimental investigations of factors controlling DNAPL transport and dissolution in fractured shale saprolite. MS Thesis. University of Tennessee. Knoxville, TN.

Project: 55196

Title: In Situ, Field Scale Evaluation of Surfactant Enhanced DNAPL Recovery Using a Single-Well, Push-Pull Test

PI: Dr. Jonathan D. Istok *Institution:* Oregon State University

Publication Type: Journal

Field, J. A. & Istok, J. D. (1998). Comment on estimation of nonaqueous phase liquid-water interfacial areas in porous media following mobilization by chemical flooding. Environmental Science and Technology, 32(2), 3836-3837.

Graduate students collaborate on a field-scale evaluation of Surfactant Enhanced DNAPL Recovery using a single-well, push-pull test. [see Project #55196]

Field, J.A., & Istok, J. D. (1999). Comment on estimation of nonaqueous phase liquid-water interfacial areas in porous media following mobilization by chemical flooding. Environmental Science and Technology. 32(2), 3836-3837.

Haggerty, R., Schroth, M. H., & Istok, J. D. (1998, Mar. - Apr.). Simplified method of "push-pull" test data analysis for determining in situ reaction rate coeffecients. Ground Water. 36(2), 314-324.

Istok, J. D., Field, J. A., Schroth, M. H., Sawyer, T. E., & Humphrey, M. D. (1999). Laboratory and field investigation of surfactant sorption using single-well, "push-pull" tests. Ground Water, 37, 589-598.

Istok, J. D., Field, J. A., Schroth, M. H., Sawyer, T. E., & Humphrey, M. D. (1999, Jul. - Aug.). Laboratory investigation of surfactant-enhanced trichloroethene solubilization using single-well 'push-pull' tests. Ground Water. 37(4), 581-588.

Project: 55359

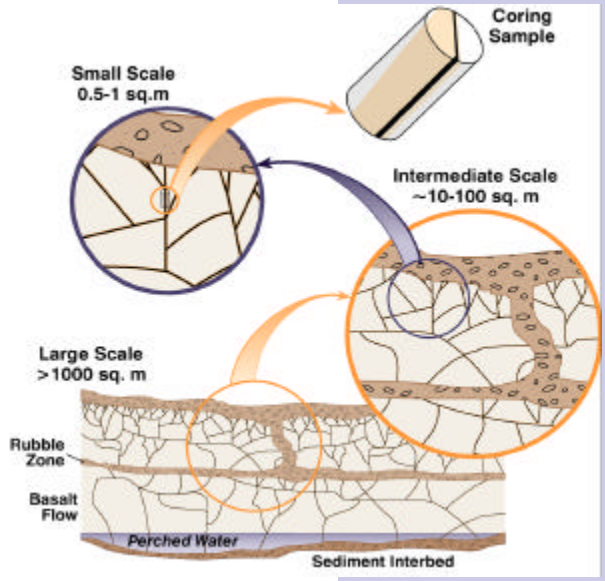
Title: Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone

PI: Dr. Boris A. Faybishenko *Institution:* Lawrence Berkeley National Laboratory

Publication Type: Journal

Finsterle, S. & Faybishenko, B. (1999). Design and analysis of an experiment to determine hydraulic parameters of variably saturated porous media. Advances in Water Resources. 22(1), 431-444.

Pruess, K., Faybishenko, B., & Bodvarsson, G. S. (1999). Alternative concepts and approaches for modeling flow and transport in thick unsaturated zones of fractured rocks. Journal of Contaminant Hydrology-Special Issue. 38, 281-322.



A four-level hierarchy of scales of hydrogeological components in fractured basalt. [see Project #55359]

Publication Type: Other

Benito, P. H., Cook, P. J., Faybishenko, B., Frefield, B., & Doughty, C. (1999). Cross-well air-injection packer tests for the assessment of pneumatic connectivity in fractured, unsaturated basalt. In Amadei, Kranz, Scott, & Smeallie (Eds.). Rock Mechanics for Industry. Balkema, Rotterdam. 843-851.

Publication Type: Presentation

Carrigan, C. R, et. al. (1999). Lessons on transport and monitoring from the LLNL Vadose Zone Observatory. Proceedings of the 1999 Spring AGU Meeting. Boston, MA.

Faybishenko, B. & Finsterle, S. (1999). On the physics of tensiometry in heterogeneous soils and rocks. Proceedings of the 1999 Spring AGU Meeting. Boston, MA.

Faybishenko, B. & Geller, J. (1999). Analysis of observed chaotic data for flow through capillary tubes. Experimental Chaos Conference.

Faybishenko, B. (1998, May). Theory and numerical evaluation of the parameters of the chaotic behavior of flow in unsaturated soils and rocks. Chapman Conference on Fractal Scaling, Non-Linear Dynamics, and Chaos in Hydrologic Systems. Clemson University. Clemson, SC.

Faybishenko, B. (1998, Oct.). A fuzzy-chaotic analysis of water flow and chemical transport in unsaturated-saturated soils. 16th World Congress of Soil Science. Montpellier, France.

Faybishenko, B. (1999). On nonlinear, chaotic dynamics of flow in unsaturated fractured rocks. Fall AGU 1999 Meeting. San Francisco, CA.

Faybishenko, B. (Ed.) (1999, Feb. 10-12), Proceedings of the International Symposium Dynamics of Fluids in Fractured Rocks: Concepts and Recent Advances. Berkeley, CA.

Faybishenko, B. On nonlinear, chaotic dynamics of flow in unsaturated fractured rocks. Fall AGU 1999 Meeting. San Francisco, CA.

Faybishenko, B., et. al. (1997). Conceptual model of geometry and physics of liquid flow in unsaturated fractured basalt at Box Canyon Site. Proceedings of the 1997 Fall Meeting of AGU. San Francisco, CA.

Faybishenko, B., et. al. (1998). Multi-scale investigations of flow in fractured rocks. Proceedings of the 1998 Fall Meeting of AGU. San Francisco, CA. F377-378.

Faybishenko, B., Wood, T. R., Stoops, T. M., Doughty, C., & Jacobsen, J. (1997). A conceptual model of tracer transport in fractured basalt: Large Scale Infiltration Test revisited. Proceedings of 1997 GSA Annual Conference. Salt Lake City, UT.

Geller, J. T., Borglin, S. E., & Faybishenko, B. (1998, May). Experimental study and evaluation of dripping water in fracture models. Chapman Conference on Fractal Scaling, Non-Linear Dynamics, and Chaos in Hydrologic Systems. Clemson University. Clemson, SC.

Geller, J. T., Borglin, S. E., & Faybishenko, B. (1998). Experimental study and evaluation of dripping water in fracture models. Proceedings of the 1998 Fall Meeting of AGU. San Francisco, CA. F383.

Podgorney, R. K., Faybishenko, B., & Wood, T. (1999). Field evidence of unstable infiltration into variably saturated fractured basalt on a 1-meter scale. Fall AGU 1999 Meeting. San Francisco, CA.

Publication Type: Press release

Faybishenko, B. (1999, Dec. 17). Water travels chaotically through the ground. A Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone (see Web site: http://www.eurekalert.org/releases/ineel-wtcttg.html).

Publication Type: Proceeding

Faybishenko, B. (1999). Comparison of laboratory and field methods for determination of unsaturated hydraulic conductivity of soils. LBNL Report-42022. Proceedings of the International Conference - Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media.

Faybishenko, B. (1999). Evidence of chaotic behavior in flow through fractured rocks, and how we might use chaos theory in fractured rock hydrogeology. Proceedings of the International Symposium Dynamics of Fluids in Fractured Rocks: Concepts and Recent Advances. Berkeley, CA. 207-212.

Finsterle, S. & Faybishenko, B. (1998). What does a tensiometer measure in fractured rocks? LBNL Report-41454. Proceedings of the International Conference - Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media.

Nikravesh, M., Cox, L., Faybishenko, B., & Aminzadeh, F. (1999, Mar.). Characterization of contaminated sites using sparse well data. SPE Paper 49330.

Podgorney, R. K. & Wood, T. R. (1999). Observations of water movement in variably saturated fractured basalt and its possible implications on predictive modeling. Proceedings of the International Symposium Dynamics of Fluids in Fractured Rocks: Concepts and Recent Advances. Berkeley, CA. 300-304.

Publication Type: Report

Babchin, A. J., Faybishenko, B., Sivashinsky, G. I., Frenkel, A., & Halpern, D. (1999). A model of chaotic time evolution of a slow liquid film on an inclined plane: One-dimensional solution. LBNL Report 42884.

Benito, P., Cook, P., Faybishenko, B., Freifeld, B., & Doughty, C. (1999). Box canyon air-connectivity study. Preliminary Data Analysis, LBNL Report 42359. CRWMS M&O 2000. Natural analogs for the unsaturated zone. MDL-NBS-HS-000007. Las Vegas, NV.

Faybishenko, B. (1999, Jun. 6-11). Short-term and long-term vadose zone monitoring: Current technologies, development, and applications. Subsurface Remediation: Improving Long-Term Monitoring & Remedial Systems Performance. LBNL Report 43408.

Faybishenko, B., et al. (1997). A chaotic-dynamical conceptual model to describe fluid flow and contaminant transport in a fractured vadose zone. Environmental Management Science Program Awards Fiscal Year 1997 Annual Report Progress. Lawrence Berkeley National Laboratory Report, LBNL-41192.

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Faybishenko, B., et. al. (1999). Conceptual model of the geometry and physics of water flow in a fractured basalt vadose zone: Box Canyon site, Idaho. LBNL Report 42915.

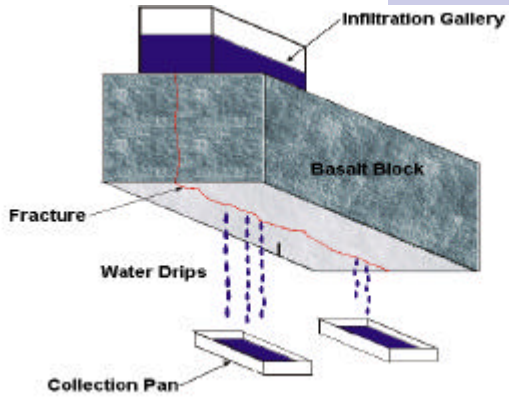

Illustration of the infiltration test design at the Hell's Half Acre site, Idaho, to investigate a key problem of infiltration in fractured rocks - water dripping through fractures. [see Project #55359]

Podgorney, R. K., Whitmire, D. L., Wood, T. R., & Stoops, T. M. (1999). Basalt outcrop infiltration tests to evaluate chaotic behavior of unsaturated flow in fractured rock, Data Summary Report, 1999 Field Season (Draft). INEEL/EXT-99-01204.

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Pruess, K., Faybishenko, B., & Bodvarsson, G. S. (1997). Alternative concepts and approaches for modeling unsaturated flow and transport in fractured rocks. Chapter 24 of The Site-Scale Unsaturated Zone Model of Yucca Mountain, Nevada, for the Viability Assessment.

Project: 60158

Title: Development of Radon-222 as a Natural Tracer for Monitoring the Remediation of NAPL Contamination in the Subsurface

PI: Dr. Lewis Semprini *Institution:* Oregon State University

Publication Type: Journal

Semprini, L., Hopkins, O. S., & Tasker, B. R. (2000, Jan.). Laboratory, field, and modeling studies of radon-222 as a natural tracer for monitoring NAPL contamination. Transport Porous Med. 38(1-2), 223-240.

Publication Type: Other

Semprini, L., Cantaloub, M., Gottipati, S., Hopkins, O., & Istok, J. (1998). Radon-222 as a natural tracer for quantifying and monitoring NAPL remediation. Wickramanayake, G. B. & Hinchee, R. E. (Eds.), Nonaqueous-phase Liquids: Remediation of Chlorinated and Recalcitrant Compounds. Battelle Press, Columbus, OH. 137-142.

Publication Type: Presentation

Cantaloub, M. (1998, Nov. 16-19). The role of cocktail solvent on radon measurement by liquid scintillation analysis. Packard Instrument Co. Environmental LSC Workshop at the 44th Annual Conference on Bioassay, Analytical, and Environmental Radiochemistry. Albuquerque, NM.

Cantaloub, M., Higginbotham, J., Istok, J. & Semprini, L. (1998, Nov. 16-19). Interaction of sample, cocktail and headspace volume when measuring aqueous Rn in small volume samples. 44th Annual Conference on Bioassay, Analytical, and Environmental Radiochemistry. Albuquerque, NM.

Cantaloub, M., Humphrey, M., Istok, J., & Semprini, L. (1998, Dec. 6-10). Monitoring NAPL remediation using Rn-222 as an in-situ indicator. 1998 Fall Meeting of the American Geophysical Union. San Francisco, CA.

Cantaloub, M., Istok, J., & Semprini, L. (1998, Dec. 1-3). Radon-222 as a natural tracer for monitoring the remediation of NAPL contamination in the subsurface. Strategic Environmental Research and Development Program (SERDP) and Environmental Security Technology Certification Program (ESTCP) Technical Symposium and Workshop. Arlington, VA.

Cantaloub, M., Istok, J., & Semprini, L. (1998, Jul. 20-23). Investigations of Radon-222 as an internal tracer for monitoring NAPL remediation. Symposium on Environmental Models and Experiments Envisioning Tomorrow; Behavior and Remediation of Nonaqueous Phase Liquid Contaminants in the Subsurface. UC Irvine, CA.

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Project: 70149 (Renewal of Project No. 54950)

Title: The Dynamics of Vadose Zone Transport: A Field and Modeling Study Using the Vadose Zone Observatory

PI: Dr. Charles R. Carrigan *Institution:* Lawrence Livermore National Laboratory

Publication Type: Journal

Carrigan, C. R. & Nitao, J. J. (2000). Predictive and diagnostic simulation of in situ electrical heating in contaminated, low-permeability soils. Cover article for Environmental Science & Technology. 34, 4835-4841.

Publication Type: Other

Carrigan, C. R. (1999). Calibration and testing of predictive models of gas-phase transport in the vadose zone: An example from the Nevada Test Site in EM sponsored book - Vadose Zone, Science and Technology Solutions. Battelle Press.

Carrigan, C. R. (1999). Understanding the fate and transport of multiphase fluid and colloidal contaminants in the vadose zone using an intermediate-scale field experiment in EM sponsored book - Vadose Zone, Science and Technnology Solutions. Battelle Press.

Publication Type: Presentation

Carrigan, C. R. & Hudson, G. B. (1998). Characterization of contaminant transport by gravity, capillary, and barometric pumping in heterogeneous vadose regimes. Extended Abstract Volume (144), DOE/EMSP Program Review. Chicago, IL.

Carrigan, C. R., et. al. (1998). The vadose zone observation: Dynamic charaterization of liquid- and gas-phase contaminant transport in a heterogenerous soil regime. Transactions of the AGU (EoS). 79(45), F384.

Carrigan, C. R., et. al. (1998, May). The vadose zone observatory: Monitoring the contaminant fast track to the water table. Presentation given to LLNL visiting Environmental Programs Science Advisory Committee (EPSAC).

Carrigan, C. R., et. al. (1999, May 31-Jun. 4). Lessons about transport and monitoring at the vadose zone observatory at LLNL. Appeared Transactions of the AGU (EoS), Spring Meeting. Boston, MA.

Ekwurzel, B., et. al. (1999, May 31-Jun. 4). Deuterium, Br, I, and 18O used as tracers of infiltration water movement throught the vadose zone. Appeared Transactions of the AGU (EoS), Spring Meeting. Boston, MA.

Hudson, G. B. (1997, Apr. 5). Isotope tracers for tracking groundwater recharge. California Water Reuse Association, Artificial Water Recharge Workshop. Newport Beach, CA.

Hudson, G. B. (1997, Jun. 10-11). The Xe-124 water infiltration experiment at Anaheim Lake. Santa Ana River Quality and Health Effects Study. Orange County Water District. Fountain Valley, CA.

Ralston, D. K., et. al. (1999, May 31-Jun. 4). Implications of modeling for gas-phase transport at the LLNL vadose zone observatory. Appeared Transactions of the AGU (EoS), Spring Meeting. Boston, MA.

Project: 70193

Title: Influence of Clastic Dikes on Vertical Migration of Contaminants in the Vadose Zone at Hanford

PI: Dr. Christopher J. Murray *Institution:* Pacific Northwest National Laboratory

Publication Type: Presentation

Fayer, M. J., et. al. (2000, Dec. 15). Hydrogeological measurements and hydrofacies models of clastic dikes at the Hanford Site, Southcentral Washington. EOS Trans. American Geophysical Union Fall Meeting. San Francisco, CA. 81(48), F412.

Murray, C., et. al. (2000, Sept. 24-27). Hydrogeological measurements and hydrofacies models of clastic dikes at the Hanford Site, Southcentral Washington. SEPM/IAS Research Conference on Environmental Sedimentology: Hydrogeology of Sedimentary Aquifers. Santa Fe, NM.

Project: 73732 (Renewal of Project No. 54680)

Title: Migration and Entrapment of DNAPLs in Heterogeneous Systems: Impact of Waste and Porous Medium Composition

PI: Dr. Linda M. Abriola *Institution:* University of Michigan

Publication Type: Journal

Bradford, S. A. & Abriola, L. M. (2001). Dissolution of residual tetrachloroehtylene in fractional wettability porous media: Incorporation of interfacial area estimates. Water Res. Res. 37(5), 1183-1195.

Bradford, S. A., Abriola, L. M., & Leij, F. J. (1997). Wettability effects on two- and three- fluid relative permeabilities. Journal of Contam. Hydrol. 28, 171-191.

Bradford, S. A., Abriola, L. M., & Rathfelder, K. M. (1998). Flow and entrapment of dense nonaqueous phase liquids in physically and chemically heterogeneous aquifer formations. Adv. Water Res. 22, 117-132.

Bradford, S. A., Vendlinski, R. A., & Abriola, L. M. (1999, Oct.). The entrapment and long-term dissolution of tetrachloroethylene in fractional wettability porous media. Water Resour. Res. 35(10), 2955-2964.

Lord, D. L., Demond, A. H., Salehzadeh, A., & Hayes, K. F. (1997). Influence of organic acid solution chemistry on subsurface transport properties. 2. Capillary pressure- saturation. Environ. Sci. Technol. 31, 2052-2058.

Lord, D. L., Hayes, K. F., Demond, A. H., & Salehzadeh, A. (1997). Influence of organic acid solution chemistry on subsurface transport properties. 1. Surface and interfacial tension. Environ. Sci. Technol. 31, 2045-2051.

Salehzadeh, A. & Demond, A. H. (1999, Apr.). Pressure cell for measuring capillary pressure relationships of contaminated sands. J. Environ. Eng-Asce. 125(4), 385-388.

Publication Type: Other

Lord, D. L., Demond, A. H., Hayes, K. F., & Salehzadeh, A. (1998). Effects of surfactant chemistry on interfacial tension, wettability, and capillary pressure in multiphase subsurface systems. Chrysikopoulos, C. V., Bear, J., & Harmon, T. C. (Eds.). Enviromeet 98- Behavior and Remediation of Nonaqueous Phase Contaminants in the Subsurface. University of California at Irvine. Irvine, CA.

Publication Type: Paper

Bradford, S. A., & Abriola, L. M. (1998). Entrapment and dissolution of organic liquids in chemically heterogeneous porous media. IAHS Publication no. 250, Groundwater Quality: Remediation and Protection. Tubingen, Germany. 167-172.

Publication Type: Presentation

Bradford, S. A., Abriola, L. M., & Rathfelder, K. M. (1997). The impact of fractional wettability and grain size distribution on the long-term dissolution of residual tetrachloroethylene. Eos, Transactions, American Geophysical Union. 78(17), 78:S158-159.

Bradford, S. A., Abriola, L. M., & Rathfelder, K. M. (1997). The impact of fractional wettability and grain size distribution on the long-term dissolution of residual tetrachloroethylene. Eos, Transactions, American Geophysical Union. 78(46), 78:F331.

Bradford, S. A., Abriola, L. M., Demond, A. H., & Lord, D. L. (1999, Aug. 22-26). Migration and entrapment of DNAPLs in chemically heterogeneous aquifer environments. American Chemical Society, National Meeting. New Orleans, LA.

Echols, R. T. & Demond, A. H. (1999). Impact of soil organic matter on the transport of organic liquids in soil. Midwest Environmental Chemistry Workshop. Houghton, MI.

Lord, D. L., Demond, A. H., & Hayes, K. F. (1997). The impact of solution chemistry on capillary pressure-saturation relationships for two-phase systems containing solutes. Eos, Transactions, American Geophysical Union. 79(45), 97:H41E-08.

Lord, D. L., Demond, A. H., & Hayes, K. F. (1998, Apr. 20-24). The impact of speciation, partitioning, and sorption on the migration of multiple fluid phases in the subsurface. European Geophysical Society Hydrology and the Earth's Crust Symposium, XXIII General Assembly. Nice, France.

Lord, D. L., Demond, H., & Hayes, K. F. (1998, Oct. 16-18). Effects of solute chemistry on soil transport properties. 21st Midwest Environmental Workshop. Ann Arbor, MI.

Lord, D. L., et. al. (1998). Impacts of organic acid and base solution and interfacial chemistry on NAPL transport in the subsurface. Eos, Transactions, American Geophysical Union. 79(45), 79:F247.

Lord, D. L., Hayes, K. F., & Demond, A. H. (1997, Apr. 13-17). The impacts of solution and interfacial chemistry on organic liquid migration in the subsurface. American Geochemical Society, National Meeting. San Francisco, CA.

O'Carroll, D. M., Bradford, S. A., & Abriola, L. M. (2000, Sep. 27-28). Infiltration and redistribution of PCE in a system containing spatial wettability variations. 6th International Symposium on Evaluation of Reservoir Wettability and Its Effect on Oil Recovery. Socorro, NM.

Phelan, T. J., O'Carroll, D. M., Bradford, S. A., & Abriola, L. M. (2000). Evaluation of DNAPL transport parameters in fractionally wet porous media. Eos, Transactions, American Geophysical Union. 81(48), H71B-07.

Publication Type: Proceeding

Bradford, S. A., Abriola, L. M., & Leij, F. J. (1999, in press). Multi-fluid hydraulic properties for fractional wettability porous media. In Van Genuchten, M. Th., Leij, F. J., & Wu, L. (Eds.), Characterization and Measurement of the Hydraulic Properties for Unsaturated Porous Media, University of California. Riverside, CA.

Bradford, S. A., Abriola, L. M., & Rathfelder, K. M. (1998). Simulated entrapment and dissolution of organic liquids in chemically heterogeneous porous media. Chrysikopoulos, C. V., Bear, J., & Harmon, T. C. (Eds.), Enviromeet 98- Behavior and Remediation of Nonaqueous Phase Contaminants in the Subsurface. University of California. Irvine, CA. 7-16.

Demond, A.H., Hayes, K. F., Lord, D. L., Desai, F., & Salehzadeh, A. (1999). Impact of organic compound chemistry on capillary pressure relationships of sands. Van Genuchten, M.Th., Leij, F. J., & Wu, L. (Eds.), Characterization and Measurement of the Hydraulic Properties for Unsaturated Porous Media. University of California. Riverside, CA. 229-240.

Lord, D. L., Demond, A. H., Hayes, K. F., & Salehzadeh, A. (2000, Jan.). Effects of organic base chemistry on interfacial tension, wettability, and capillary pressure in multiphase subsurface waste systems. Transport. Porous. Med. 38(1-2), 79-92.

Publication Type: Theses/Dissertations

Lord, D. L. (1999). Influence of organic acid and base solution chemistry on interfacial and transport properties of mixed wastes in the subsurface. Ph.D. dissertation. Department of Civil and Environmental Engineering, The University of Michigan. Ann Arbor, MI.

Project: 73812 (Renewal of Project No. 55395)

Title: Physics of DNAPL Migrations and Remediation in the Presence of Heterogeneities

PI: Dr. Stephen H. Conrad *Institution:* Sandia National Laboratories - Albuquerque

Publication Type: Report

Borchers, B., Conrad, S. H., Webb, E. K., Glass Jr., R. J., Cox, R. (1997). A simulation and decision analysis approach to locating DNAPL in subsurface sediments. Sandia Report SAND97-2261.

Inorganic Chemistry

Project: 54834

Title: An Investigation of Homogeneous and Heterogeneous Sonochemistry for Destruction of Hazardous Waste

PI: Dr. Inez Hua *Institution:* Purdue University

Publication Type: Journal

Beckett, M. A. & Hua, I. (2000). Elucidation of the 1,4-dioxane decomposition pathway at discrete ultasonic frequencies. Environmental Science and Technology. 34(19), 3944-3953.

Hoffmann, M. R., Hua, I., & Hochemer, R. (1996). Application of ultrasonic irradiation for the degradation of chemical contaminants in water. Ultrasonics Sonochemistry. 3(3), 163-172.

Hua, I. & Hoffmann, M. R. (1996). Kinetics and mechanism of the sonolytic degradation of CCl4: Intermediates and by-products. Environmental Science and Technology. 30(3), 864-871.

Hua, I. & Hoffmann, M. R. (1997). Sonochemical production of hydroxyl radical and hydrogen peroxide: The effect of frequency and saturating gas. Environmental Science and Technology. 31(8), 2237-2243.

Hua, I. & Thompson, J. (2000). Inactivation of escherichia coli by sonication at discrete ultrasonic frequencies. Water Research. 34(15), 3888-3893.

Hua, I. & Zhang, G. M. (1999, Mar. 21). Cavitation chemistry of polychlorinated biphenyls. Abstr. Pap. Am. Chem. S. 217, U623-U623, Part 1.

Hua, I., Hochemer, R. H., & Hoffman, M. R. (1995). The sonochemical degradation of p-nitrophenol in a parallel-plate near-field acoustical processor. Environmental Science and Technology. 29(11), 2790-2796.

Hua, I., Hochemer, R. H., & Hoffmann, M. R. (1995). Sonolytic hydrolysis of p-nitrophenylacetate: The role of supercritical water. Journal of Physical Chemistry. 99(8), 2335-2342.

Schramm, J. & Hua, I. (2000). Ultrasonic irradiation of dichlorvos: Decomposition mechanism and mass balances. Water Research. 35(3), 665-674.

Weavers, L. K., Hua, I., & Hoffmann, M. R. (1997). A new advanced oxidation process: Photoassisted oxidation of triethanolamine by periodate. Water Environment Research. 69(6), 1112-1119.

Zhang, G. & Hua, I. (2000). Ultrasonic degradation of trichloroacetonitrile, chloropicrin, bromobenzene: Design factors and matrix effects. Advances in Environmental Research. 4(1), 211-218.

Zhang, G. M. & Hua, I. (2000, Apr. 15). Cavitation chemistry of polychlorinated biphenyls: Decomposition mechanisms and rates. Environ. Sci. Technol. 34(8), 1529-1534.

Publication Type: Presentation

Hua, I. (1999, Feb.). The use of ultrasonic irradiation in environmental engineering processes. Borchardt Conference, The University of Michigan. Ann Arbor, MI.

Pfalzer, U. & Hua, I. (1997, Nov. 9). Sonochemical degradation of carbofuran in a parallel-plate near-field acoustical processor. 20th Annual Midwest Environmental Chemistry Workshop, Indiana University. Bloomington, IN.

Schramm, J. & Hua, I. (1997, Sept.). Degradation of dichlorvos by sonolysis. American Chemical Society Meeting. Las Vegas, NV.

Zhang, G. & Hua, I. (1998, Mar.). Destruction of polychlorinated biphenyls in acoustically cavitating systems. American Chemical Society Meeting. Dallas, TX.

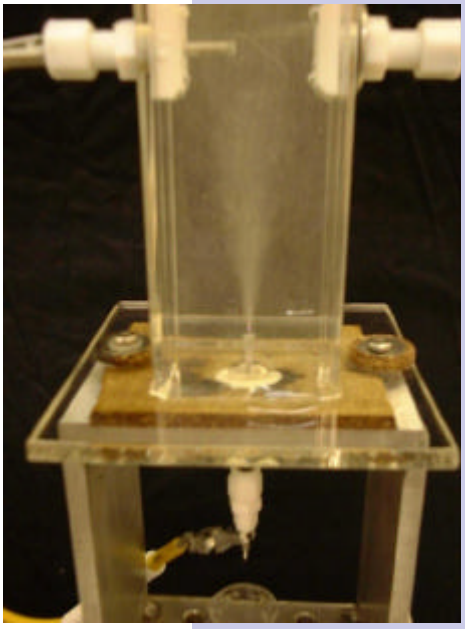
Project: 55119

Title: Phase Equilibria Modification by Electric Fields
PI: Dr. Costas Tsouris
Institution: Oak Ridge National Laboratory

Publication Type: Journal

Blankenship, K. D., DePaoli, D. W., Hylton, J. O., & Tsouris, C., (1999). Effect of electrode configurations on phase equilibria with electric fields. Separation and Purification Technology. 15, 283-294.

Blankenship, K. D., Shah, V. M., & Tsouris, C. (1999). Distillation under electric fields. Separation Science and Technology. 34, 1393-1409.



Simultaneous pumping, spraying, and mixing of a gas in an aqueous solution by means of an electric field can be used for the removal of contaminants from the solution. [see Project #55119]

Norato, M. A., Tsouris, C., & Tavlarides, L. L. (1998). Phase inversion studies in liquid-liquid dispersions. The Canadian Journal of Chemical Engineers. 76, 486-494.

Shin, W-. T., Yiacoumi, S., & Tsouris, C. (1997). Experiments on electrostatic dispersion of air in water. Industrial and Engineering Chemistry Research. 36, 3647-3655.

Starkweather, B. A., Connell, B. L., & Counce, R. M. (1998, Jul.). Experimental effects help cleaning success. Precision Cleaning. 5(7).

Starkweather, B. A., Zhang, X. G., & Counce, R. M. (2000). An experimental study of the change in the contact angle of an oil on a solid surface. Industrial and Engineering Chemistry Research.

Tsouris, C. & Dong, J. (2000). Effects of electric fields on phase inversion of liquid-liquid dispersions. Chemical Engineering Science. 55, 3571-3574.

Tsouris, C., Shin, W.- T., Yiacoumi, S., & DePaoli, D. W. (2000, in press). Effects of electric fields on bubble and particle velocities in water and alcohols. Journal of Colloid and Interface Science.

Tsouris, C., & Dong, J. H. (2000, Sept.). Effects of electric fields on phase inversion of liquid-liquid dispersions. Chemical Engineering Science. 55(17), 3571-3574.

Tsouris, C., Borole, A. P., & Kaufman, E. N., DePaoli, D. W. (1999). An electrically driven gas-liquid-liquid contactor for bioreactor and other applications. Industrial and Engineering Chemistry Research. 38, 1877-1883.

Tsouris, C., DePaoli, D. W., Shor, J. T., Hu, M. Z.- C., & Ying, T. -Y. (2000). Electrocoagulation for magnetic seeding of colloidal particles. Colloids and Surfaces, 177, 227-237.

Tsouris, C., Shin, W.- T. & Yiacoumi, S. (1998). Pumping, spraying, and mixing of fluids by electric fields. The Canadian Journal of Chemical Engineers. 76, 589-599.

Tsouris, C., Shin, W.-T., Yiacoumi, S., & DePaoli, D. W. (2000). Electrohydrodynamic velocity measurements in water and alcohols. Journal of Colloid and Interface Science. 229, 335-345.

Publication Type: Paper

Tsouris, C., & Dong, J. (1999, Jun. 13-16). Electric-field effects on fluid interfaces. 73rd ACS Colloid and Surface Science Symposium, Massachusetts, Institute of Technology. Cambridge, MA.

Publication Type: Patent

DePaoli, D. W. & Tsouris, C. (1999). Continuous flow, electrohydrodynamic micromixing apparatus and methods. Patent Application No. 09/398,675.

DePaoli, D. W. & Tsouris, C. (1999). Continuous flow, electrohydrodynamic micromixing apparatus and methods. Application No. 09/398,675.

Tsouris, C. & Dong, J. (1999). Methods to control phase inversions and enhance mass transfer in liquid-liquid dispersions. Patent Application No. 09/397,281.

Tsouris, C. & Dong, J. (1999). Methods to control phase inversions and enhance mass transfer in liquid-liquid dispersions. Application No. 09/397,281.

Tsouris, C., DePaoli, D. W., & Shor, J. T. (1999). A method to electrolytically produce high-purity magnetite powder. Application No. 09/371,638.

Tsouris, C., DePaoli, D. W., & Shor, J. T. (1999). A method to electrolytically produce high-purity magnetite powder. Patent Application No. 09/371,638.

Publication Type: Presentation

Blankenship, K. D., DePaoli, D. W., Hylton, J. O., & Tsouris, C. (1998, Nov. 15-20). Distillation with applied electric fields. AIChE Annual Meeting, Miami, FL.

Blankenship, K. D., Shah, V. M., & Tsouris, C. (1997, Oct. 20-24). Distillation under electric fields. Tenth Symposium on Separation Science and Technology for Energy Applications, Gatlinburg, TN.

DePaoli, D. W., Tsouris, C., & Hu, M. Z.- C. (1999, Aug. 15-20). Electrohydrodynamic mixing and reaction in multiphase and miscible systems. MIXING XVII, Banff, Canada.

Dong, J. & Tsouris, C. (1999, Oct. 17-20). A novel solvent extraction approach using electric fields. Eleventh Symposium on Separation Science and Technology for Energy Applications, Gatlinburg, TN.

Dong, J. & Tsouris, C. (1999, Oct. 31-Nov. 5). Effect of electric fields on phase inversion in liquid-liquid dispersions. AIChE Annual Meeting, Dallas, TX.

Perkins, L., Fu, B., Counce, R. M., DePaoli, D., & Hu, M. (1999). Phase separation of oil/water emulsions in the presence of surfactants. 11th Symposium on Separation Science and Technology for Energy Applications. Gatlinburg, TN.

Rowe, A., Counce, R. M., DePaoli, D., & Hu, M. (1999). pH effects on adsorption aqueous surfactants. 11th Symposium on Separation Science and Technology for Energy Applications. Gatlinburg, TN.

Tsouris, C. (1997, Jul.). Status and directions in electroseparations. EPRI Chemicals & Petroleum Target Strategic Research Meeting, Electric Power Research Institute, Palo Alto, CA.

Tsouris, C. (1998, Feb.). Pumping, spraying, and mixing of fluids by electric fields. School of Civil and Environmental Engineering, Georgia Institute of Technology.

Tsouris, C. (1999, Oct.). Electrohydrodynamic micromixing reactors. Department of Chemical Engineering, Auburn University.

Tsouris, C., Blankenship, K. D., DePaoli, D. W., Shin, W.- T., & Hylton, J. O. (1998, Jun. 21-24). Electric-field effects on gas-liquid and liquid-liquid systems. 72nd Colloid and Surface Science Symposium,

Tsouris, C., Blankenship, K. D., Dong, J., & DePaoli, D. W. (1999, Oct. 17-20). Distillation with electric fields. Eleventh Symposium on Separation Science and Technology for Energy Applications, Gatlinburg, TN.

Tsouris, C., DePaoli, D. W., & Yiacoumi, S., (1999, Jun. 1). Novel environmental technologies driven by electric and magnetic fields. Environmental Technologies and Opportunities Forum. Oak Ridge, TN.

Tsouris, C., DePaoli, D. W., Shor, J. T., Hu, M. Z.- C., & Ying, T.- Y. (1998, Jun. 21-24). Electrochemical methods for magnetic seeding of wastewaters. 72nd Colloid and Surface Science Symposium, University Park, Pennsylvania State University, State College, PA.

Tsouris, C., Dong, J., & DePaoli, D. W. (1999, Aug. 15-20). Novel phenomena in liquid-liquid systems under the influence of electric fields. MIXING XVII, Banff, Canada.

Tsouris, C., et. al. (1998, Jul. 27-30). Phase equilibria modification by electric fields. Environmental Management Science Program National Workshop, Chicago, IL.

Tsouris, C., Shin, W. -T., & Yiacoumi, S. (1997, Jun. 29-Jul. 2). Formation of microbubbles using electric fields for environmental applications. 71st Colloid and Surface Science Symposium, Newark, DL.

Worden, R. M., Bredwell, M. D., & Tsouris, C. (1998, May 3-7). Synthesis gas fermentations: Mass transfer improvement in butyribacterium methylotrophicum fermentations. 20th Symposium on Biotechnology for Fuels and Chemicals.

Yiacoumi, S., Ying, T.- Y., Yang, K.- L., & Tsouris, C. (1999, Oct. 31-Nov. 5). Electrosorption of metal ions from aqueous solutions. AIChE Annual Meeting, Dallas, TX.

Ying, T.- Y., Yang, K.- L., Yiacoumi, S., & Tsouris, C. (1999, Oct. 17-20). Electrosorption of metal ions from aqueous solutions. Eleventh Symposium on Separation Science and Technology for Energy Applications, Gatlinburg, TN.

Ying, T.- Y., Yiacoumi, S., Tsouris, C., Shor, J. T., & DePaoli, D. W. (1999, Oct. 17-20). Electrocoagulation, magnetic seeding, and high-gradient magnetic filtration. Eleventh Symposium on Separation Science and Technology for Energy Applications, Gatlinburg, TN.

Publication Type: Theses/Dissertations

Blankenship, K. D. (1999, Apr.). Distillation with applied electric fields. Masters Thesis, Department of Chemical Engineering, University of Tennessee. Knoxville, TN.

Shin, W.- T. (2000). Electric-field enhanced separations. PhD dissertation. Georgia Institute of Technology.

Yang, K.- L. (2002). Electrosorption modeling of equilibrium and kinetics. Georgia Institute of Technology.

Ying, T.- Y. (2001). Electrosorption of metal ions from aqueous solution. Georgia Institute of Technology.

Microbial Science

Project: 54681

Title: Dynamics of Coupled Contaminant and Microbial Transport in Heterogeneous Porous Media

PI: Dr. Timothy R. Ginn *Institution:* University of California at Davis

Publication Type: Journal

VanSchie, P. M., Boone, D. R., & Fletcher, M. (1999). Adhesion of biodegradative anaerobic bacteria to solid surfaces. Appl. Env. Microbial. 65, 5082-5088.

Publication Type: Poster

VanSchie, P. M. & Fletcher, M. (1999). Characterization of the adhesive behavior of anaerobic bacteria with bioremediation potential. Amer. Soc. Microb. 131/Q Q-164.

VanSchie, P. M., Boone, D. R., & Fletcher, M. (1998). Adhesion of biodegradative anaerobic bacteria to solid surfaces. Amer. Soc. Microb. 118/Q Q-60.

Project: 55031

Title: Genetic Analysis of Stress Responses in Soil Bacteria for Enhanced Bioremediation of Mixed Contaminants

PI: Dr. Kwong-Kwok Wong *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Markillie, L. M., Varnum, S., Hradecky, P., & Wong, K. K. (1999). Targeted mutagenesis by duplication insertion in the radioresistant bacterium Deinococcus radiodrans: Radiation sensitivities of catalase (katA) and superoxide dismutase (sodA) mutants. Journal of Bacteriology. 181, 666-669.

Romine, M., et. al. (1999). Complete sequence of a 184.5-kb. catabolism plasmid from Sphingomonas aromaticivorans strain F199. Journal of Bacteriology. 181, 1585-1602.

Wong, K. K., Markillie, L. M., & Saffer, J. D. (1997). A novel method for producing partial restriction digestion of DNA fragments by PCR with 5-methyl-dCTP. Nucleic Acids Res. 25, 4169-4171.

Wong, K. K., Stillwell, L. C., Dockery, C. A., & Saffer, J. D. (1996). Use of tagged random hexamer amplification (THRA) to clone and sequence minute quantities of DNA-application to a 180-kb. plasmid isolated from Sphingomonas F199. Nucleic Acids Res. 24, 3778-3783.

Project: 55105

Title: Complete Detoxification of Short Chain Chlorinated Aliphatics: Isolation of Halorespiring Organisms and Biochemical Studies of the Dehalogenating Enzyme Systems

PI: Dr. James M. Tiedje *Institution:* Michigan State University

Publication Type: Journal

Löffler, F. E., Ritalahti, K. M., & Tiedje, J. M. (1997). Dechlorination of chloroethenes is inhibited by 2-bromoethanesulfonate in the absence of methanogens. Appl. Environ. Microbiol. 63, 4982-4985.

Löffler, F. E., Sun, Q., Li, J., & Tiedje, J. M. (2000, in press). PCR detection of desulfuromonas and dehalococcoides, two environmentally important groups of tetrachloroethene (PCE)-dechlorinating anaerobic bacteria. Appl. Environ. Microbiol.

Löffler, F. E., Tiedje, J. M., & Sanford, R. A. (1999). The fraction of electrons consumed in electron acceptor reduction (FE) and hydrogen thresholds as indicators of halorespiratory physiology. Appl. Environ. Microbiol. 65, 4049-4056.

Project: 55152

Title: Molecular Profiling of Microbial Communities from Contaminated Sources: Use of Subtractive Cloning Methods and rDNA Spacer Sequences

PI: Dr. Frank T. Robb *Institution:* University of Maryland at Baltimore

Publication Type: Journal

Spiro, A., Lowe, M., & Brown, D. (2000). A bead-based method for multiplexed identification and quantification of DNA sequences using flow cytometry. Appl. Environ. Microbiology 66(10), 4258-4265.

Project: 55416

Title: Control of Biologically Active Degradation Zones by Vertical Heterogeneity: Applications in Fractured Media

PI: Dr. Frederick S. Colwell *Institution:* Idaho National Engineering and Environmental Laboratory

Publication Type: Journal

Lehman, R. M., Colwell, F. S., & Bala, G. A. (2001). Attached and unattached microbial communities in a simulated basalt aquifer under fracture- and porous-flow conditions. Appl. Environ. Microbiol. 67, 2799-2809.

During a tour of the INEEL Research Center labs, INEEL scientist Rick Colwell explained to DOE Deputy Secretary T.J. Glautheir, DOE-Idaho Manager Bev Cook, Merna Hurd, senior adviser for Glautheir, and Linda McCoy, DOE chief scientist, Environemntal Management Science Program funded research into remediating the TAN aquifer using microbes, and what controls microorganisms that are degrading contaminants inthe aquifer. [see Project #55416]

Tobin, K. J., Colwell, F., Onstott, T. C., & Smith, R. (2000). Recent calcite spar in an aquifer waste plume: A possible example of contamination driven calcite precipitation. Chem. Geol. 169, 449-460.

Tobin, K. J., Onstott, T. C., Deflaun, M., Colwell, F., & Fredrickson, J. (1999). In situ imaging of microorganisms in geologic material. J. Microbiol. Meth. 37, 201-213.

Publication Type: Other

Colwell, F. (2001). Constraints on the distribution of microorganisms in subsurface environments. Fredrickson, J. & Fletcher, M. (Eds.). Subsurface Microbiology and Biogeochemistry. John Wiley and Sons. New York, NY.

Publication Type: Poster

Colwell, F. S. (1999, Jan. 15). Control of biologically active degradation zones by vertical heterogeneity: Applications in fractured media. NABIR Investigator's Workshop.

Publication Type: Presentation

Colwell, F. S. (1999). Chaotic-dynamical conceptual model to describe fluid flow and contaminant transport in a fractured vadose zone. Poster presentation at the Berkeley Dynamics of Fluids and Fractured Rock Conference. Berkeley, CA.

Understanding the chemical and microbial conditions in the subsurface helps identify potential treatment solutions. [see Project #55416]

Colwell, F. S., Tobin, K., & Wilson, M. (1999, Jan. 7). Control of biologically active degradation zones by vertical heterogeneity: Applications in fractured media. Idaho Water Resources Research Institute (IWRRI) meeting.

Publication Type: Proceeding

Lehman, R. M., O'Connell, S. P., Garland, J. L., & Colwell, F. S. (1997). Evaluation of remediation by community-level physiological profiles. Insam, H. & Rangger, A. (Eds.). Microbial Communities: Functional Versus Structural Apporaches. Springer-Verlag. Berlin, Germany.

O'Connell, S. P., Lehman, R. M., Colwell, F. S., & Watwood, M. E. (1997). Microbiological monitoring of contaminants in a fractured basalt aquifer. In Situ and On-site Bioremediation, Vol. 4. The Fourth International Symposium. Batelle Press. Columbus, OH. 111-116.

Publication Type: Theses/Dissertations

Lehman, R. M. (2000). Attached and unattached microbial communities in saturated terrestrial subsurface environments. Ph. D. Dissertation. Idaho State University. Pocatello, ID.

Project: 59786

Title: Design and Construction of *Deinococcus radiodurans* for Biodegradation of Organic Toxins at Radioactive DOE Waste Sites

PI: Dr. Michael J. Daly *Institution:* Uniformed Services Univ. of the Health Sciences

Publication Type: Journal

Brim, H., et. al. (2000, Jan.). Engineering Deinococcus radiodurans for metal remediation in radioactive mixed waste environments. Nat. Biotechnol. 18(1), 85-90.

Daly, M. J. (2000). Engineering radiation-resistant bacteria for environmental biotechnology. Current Opinion in Biotechnology. 11, 280-285.

Frederickson, J. K., Kostandarithes, H. M., Li, A. W., Pyle, A. E., & Daly, M. J. (2000). Reduction of Fe(III), Cr(VI), U(VI), and Tc(VIII) by Deinococcus radiodurans. Appl. Environ. Microbiol. 66, 2006-2011.

Lange, C., Wackett, L., Minton, K. & Daly, M. J. (1998). Engineering a recombinant Deinococcus radiodurans for organopollutant degradation in radioactive mixed waste environments. Nature Biotech. 16, 929-933.

Lin, J., et. al. (1999, Sep. 3). Whole-genome shotgun optical mapping of Deinococcus radiodurans. Science. 285(5433), 1558-1562.

Makarova, K. S., Aravind, L., Daly, M. J., & Koonin, E. (2000, in press). Specific expansion of protein families in the radioresistant bacterium Deinococcus radiodurans. Genetica.

Makarova, K. S., Wolf, Y. I., Minton, K. W., White, O., & Daly, M. J. (1999). Short repeats and insertional elements in Deinococcus radiodurans and comparison to other bacterial species. Res. Microbiol. 150, 711-724.

Venkateswaran, A., et. al. (2000). Physiologic determinants of radiation resistance in Deinococcus radiodurans. Appl. Environ. Microbiol. 66,2620-2626.

White, O., et. al. (1999). Sequencing and functional analysis of the Deinococcus radiodurans genome. Science. 286, 1571-1577.

Plant Science

Project: 54898

Title: Molecular Dissection of the Cellular Mechanisms Involved in Nickel Hyperaccumulation in Plants

PI: Dr. David E. Salt *Institution:* Purdue University

Publication Type: Journal

Krämer, U., Pickering, I. J., Prince, R. C., Raskin, I., & Salt, D. E. (2000, Apr.). Subcellular localization and speciation of nickel in hyperaccumulator and non-accumulator Thlaspi species. Plant Physiol. 122(4), 1343-1353.

Thlaspi Goesingense growing in its native ultramafic habitat near Redschlag/Austria. The Northern Arizona University team is investigating, at the molecular level, the role of histidine biosynthesis in byperaccumulation in *Thlaspi goesingense*. [see Project #54898]

Krämer, U., Smith, R. D., Wenzel, W., Raskin, I., & Salt, D. E. (1997). The role of nickel transport and tolerance in nickel hyperaccumulation by Thlaspi goesingense Hálácsy. Plant Physiol. 115, 1641-1650.

Persans, M. W., Xiange,Y., Patnoe, J. M. M. L., Krämer, U., & Salt, D. E. (1999, Dec.). Molecular dissection of the role of histidine in nickel hyperaccumulation in Thlaspi goesingense (Hálácsy). Plant Physiol. 121(4), 1117-1126.

Persans, M., Yan, X., Smith, R., & Salt, D. E. (1998). Cloning of two cDNA's from the Ni hyperaccumulator Thlaspi goesingense: Histidinol dehydrogenase (Accession No. AF023141) and imidazolglycerol-phosphate dehydratase (Accession No. AF023140), two enzymes in the histidine biosynthetic pathway. Plant Physiol Plant Gene Register. 117, 332.
PIckering, I. J., et. al. (2000, Apr.). Reduction and coordination of arsenic in Indian mustard. Plant Physiol. 122(4), 1171-1177.

Salt, D. E., Prince, R. C., Baker, A. J. M., Raskin, I., Pickering, I. J. (1999). Zinc ligands in the metal hyperaccumulator Thlaspi caerulescens as determined using X-ray absorption spectroscopy. Environmental Science and Technology. 33, 713-717.

Salt, D. E., Smith, R. D., & Raskin, I. (1998). Phytoremediation. Ann Rev Plant Physiol Plant Mol Biol. 49, 643-668.

Publication Type: Other

Salt, D. E. (1999, in press). Phytoextraction: Present applications and future promise. Wise, D. L., Trantolo, D. J., Inyang, H. I., & Cichon, E. J. (Eds.), Remediation of Hazardous Waste Contaminated Soils, 2nd Edition, Marcel Dekker, Inc.

Salt, D. E., & Baker, A. J. M. (1999, in press). Phytoremediation of metals. Rehm, H. -J. & Reed, G. (Eds.),Biotechnology 2nd Edition, Wiley-VCH. New York, NY.

Salt, D. E., & Krämer, U. (1999, in press). Mechanisms of metal hyperaccumulation in plants. Ensley, B. D. & Raskin, I. (Eds.), Phytoremediation of Toxic Metals: Using Plants to Clean-Up the Environment, Chapter 13, John Wiley & Sons, Inc., New York, NY.

Salt, D. E., Kato, N., Krämer, U., Smith, R. D. & Raskin, I. (1999). The role of root exudates in nickel hyperaccumulation and tolerance in accumulator and non-accumulator species of Thlaspi. Terry, N. & García-España, X. (Eds.), Phytoremediation of Contaminated Soil and Water, Chapter 10, CRC Press LLC. Boca Raton, FL. 189-200.

Wenzel, W., Salt, D. E., Smith, R. D., & Adriano, D. C. (1999). Phytoremediation: A plant-microbe-based remediation system. Adriano, D. C., et. al. (Eds.), Bioremediation of Contaminated Soils. American Society of Agronomy Inc., Crop Science Society of America, Inc., Soil Science Society of America, Inc., Madison, Wisconsin. 18, 457-508.

Publication Type: Paper

Special Symposium - Phytoremediation. (1999, Jul. 11-15). Progress towards a molecular understanding of metal hyperaccumulation in plants. 5th International Conference on the Biogeochemistry of Trace Elements. Vienna, Austria.

Publication Type: Presentation

Plenary Address - Phytoremediation as a Clean-Up Technology for the Next Millennium (1999, Jun. 23-25). The Researcher's Perspective - Progress and Bottlenecks. 4th IBC Annual International Conference on Phytoremediation, Toronto, Canada.

Remediation Mini-Symposium. (1999, Jul. 24-28). Towards a molecular understanding of the mechanism of Ni hyperaccumulation in Thlaspi. American Society of Plant Physiologists Annual Meeting. Baltimore, MD.

Project: 55041

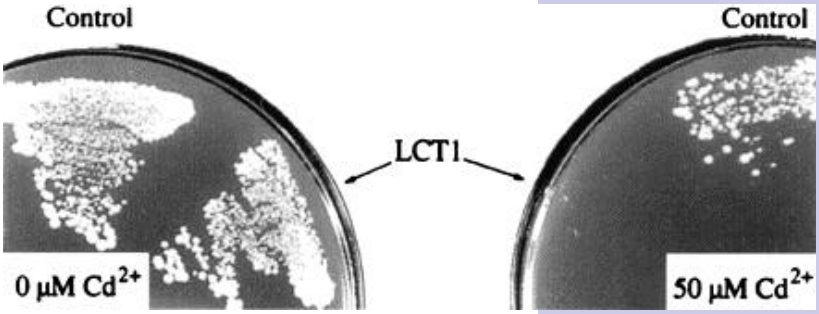
Title: Molecular Characterization of a Novel Heavy Metal Uptake Transporter from Higher Plants & its Potential for use in Phytoremediation

PI: Dr. Julian I. Schroeder

Institution: University of California at San Diego

Publication Type: Journal

Clemens, S., Kim, E. J., Neumann, D., & Schroeder, J. I. (1999). Tolerance to toxic metals by a gene family of phytochelatin synthases from plants and yeast. EMBO J. 18, 3325-3333.



LCT1 Mediates Cadmium Uptake. Expression of the wheat gene, LCT1, in *S. cerevisiae* leads to dramatic hypersensitivity to cadmium, and increased intracellular accumulation. [see Project #55041]

Project: 55097

Title: Heavy Metal Pumps in Plants
PI: Dr. Jeffrey F. Harper *Institution:* The Scripps Research Institute

Publication Type: Theses/Dissertations

Wang, Y. (2000, May). Identification of a molybenum uptake pump in arabidopsis plants. Ph.D Dissertation. Scripps Research Institute.

Project: 55278

Title: Molecular Genetics of Metal Detoxification: Prospects for Phytoremediation
PI: Dr. David W. Ow *Institution:* U.S. Dept. of Agriculture

Publication Type: Journal

Ow, D. W. (1996). Heavy metal tolerance genes: Prospective tools for bioremediation. Resources, Conservation, and Recycle. 18, 135-149.

Perego, P., VandeWeghe, J., Ow, D. W., & Howell, S. B. (1997). The role of determinants of cadmium sensitivity in the tolerance of Schizosaccharomyces pombe to cisplatin. Molecular Pharmacology. 51, 12-18.

VandeWeghe, J. & Ow, D. W. (1999). A fission yeast gene for mitochondrial sulfide oxidation. Journal of Biological Chemistry. 274, 13250-13257.

Publication Type: Other

Ow, D. W. (1998). Prospects of engineering heavy metal detoxification genes in plants. In Shewry, P. (Ed.), Engineering Crops for Industrial Uses. Portland Press. 111-124.

Picture 1 - shows a set of plants grown in high zinc concentration. Control plant (C) produces low biomass and suffers severe stress, as indicated by early flowering. In contrast, plants transgenic for genes Bj4 and Bj6 show healthy growth. [see Project #55278]

Publication Type: Presentation

Ow, D. W. (1996, Sept. 16-18). Prospects of engineering heavy metal detoxification genes in plants. Abstracts of the Symposium on Engineering Crops for Industrial End Uses. Bristol, England.

Ow, D. W. (1997, Sept. 29 - Oct. 1). Heavy metal tolerance genes as tools for phytoremediation. Abstracts of the International Symposium on Environmental Engineering. Kyongju, Korea.

Ow, D. W., Clark, S., Henstrand, J., & Kim, J. (1998, Jun. 19-20). Molecular genetics of heavy metal tolerance. Abstracts of the University of Connecticut Agricultural Biotechnology Symposium, Storrs, CN.

Ow, D. W., et. al. (1997, Sept. 21-27). Heavy metal tolerance genes for phytoremediation. Abtracts of the 5th International Congress of Plant Molecular Biology, Singapore.

Ow, D. W., et. al. (1998, Jul. 27-30). Heavy metal tolerance genes. Abstracts of the DOE Environmental Remediation Meeting. Chicago, IL.

Ow, D. W., Kim, J. H., Fox, T., & Sin, M. (2000, Apr. 25-27). Cloning heavy metal tolerance genes. Presentation at the Environmental Management Science Program National Workshop. Atlanta, GA.

VandeWeghe, J. & Ow, D. W. (1996, Aug. 6-11). An oxidoreductase-like gene required for cadmium tolerance in Schizosaccharomyces pombe. Abstracts of the 1996 Yeast Genetics & Molecular Biology Meeting. Univ. of Wisconsin. Madison, WI. 309.

VandeWeghe, J., Ow, D. W. (1997, Apr. 7-8). A novel mitochrondrial oxidoreductase required for phytochelatin accumulation and cadmium tolerance in fission yeast. Abstracts of the Society for Experimental Biology Annual Meeting, Session on Metals and Genes. Canterbury, England. 80.

Zankel, T. C. & Ow, D. (1996, Mar. 17-23). Homologs of the human BTF3 and Wiskott-Aldrich syndrome proteins are involved in the metal stress response of S. pombe. Abstracts of the 1996 Keystone Symposium on Transcriptional Mechanisms. Taos, NM. 67.

Zankel, T. C., Ow, D. W. (1997, Mar. 31 - Apr. 6). A Schizosaccharomyces pombe homolog of the Wiskott-Aldrich syndrome protein is involved in stress adaptation and mating. Abstracts of the 1997 Keystone Symposium on Temporal and Spatial Determinants of Specificity in Signal Transduction, Keystone, CO.

Publication Type: Proceeding

Perego, P, Vandeweghe, J, Ow, D, & Howell, S B. (1997). Role of determinants of cadmium sensitivity in the sensitivity of Schizosaccharomyces pombe to cisplatin. Eighty-eighth Annual Meeting of the American Association for Cancer Research, San Diego, CA. Also in the proceedings of the American Association for Cancer Research Annual Meeting. 38, 393.

Perego, P., VandeWeghe, J., Ow, D., & Howell, S. B. (1996, Apr. 20-24). Mechanisms of resistance to cisplatin (DDP) in Schizosaccharomyces pombe. 87th Annual Meeting of the American Association for Cancer Research. Washington, D. C. Proceedings of the American Association for Cancer Research Annual Meeting. 37, 336.

Publication Type: Theses/Dissertations

VandeWeghe, J. G. (1997). A mitochondrial sulfide dehydrogenase required for heavy metal tolerance in fission yeast. Ph.D. Dissertation. University of California at Berkeley. Berkeley, CA.

Project: 60271

Title: Characterization of a New Family of Metal Transport Proteins
PI: Dr. Mary Lou Guerinot *Institution:* Dartmouth College

Publication Type: Journal

Eng, B. H., Guerinot, M. L., Eide, D., & Saier, M. H. J. (1998). Sequence analyses and phylogenetic characterization of the ZIP family of metal ion transport proteins. J. Membr. Biol. 166, 1-7.

Gitan, R. S., Luo, H., Rodgers, J., Broderius, M., & Eide, D. (1998). Zinc-induced inactivation of the yeast ZRT1 zinc transporter occurs through endocytosis and vacuolar degradation. J. Biol. Chem. 273, 28617-28624.

Guerinot, M. L. & Eide, D. (1999). Zeroing in on zinc uptake in yeast and plants. Curr. Opin. Plant Biol. 2, 244-249.

Korshunova, Y. O., Eide, D., Clark, W. G., Guerinot, M. L., & Pakrasi, H. B. (1999). The IRT1 protein from Arabidopsis thaliana is a metal transporter with broad specificity. Plant Mol. Biol. 40, 37-44.

Project: 70054 (Renewal of Project No. 54837)

Title: Phytoremediation of Ionic and Methyl Mercury Pollution
PI: Dr. Richard B. Meagher *Institution:* University of Georgia

Transgenic merA9 tobacco efficiently remove mercury from hydroponic media. [see Project #70054, renewal of #54837]

Publication Type: Journal

Heaton, A. C. P., Rugh, C. L., Wang, N. -J., & Meagher, R. B. (1998). Phytoremediation of mercury and methylmercury polluted soils using genetically engineered plants. J. Soil Contam. 7, 497-509.

Rugh, C. L., Gragson, G. M., & Meagher, R. B. (1998). Toxic mercury reduction and remediation using transgenic plants with a modified bacterial gene. Hort. Sci. 33, 12-15.

Rugh, C. L., Senecoff, J. F., Meagher, R. B., & Merkle, S. A. (1998). Development of transgenic yellowpoplar for mercury phytoremediation. Nature Biotech. 16, 925-928.

Publication Type: Other

Rugh, C. L., Bizily, S. P., & Meagher, R. B. (1999). Phytoremediation of environmental mercury pollution. Ensley, B. & Raskin, I. (Eds.), Phytoremediation of toxic metals: Using plants to clean-up the environment. Wiley and Sons, New York, NY.

Publication Type: Paper

Meagher, R. B. (1998). Phytoremediation: An affordable, friendly technology to restore marginal lands in the twenty-first century. Plants and Population: Is there time? Natl. Acad. Sci. Colloquium. Irvine, CA.

Genetically altered seeds are placed in mercury-contaminated soil to see if they will grow. [see Project #70054, renewal of #54837]

Publication Type: Proceeding

Bizily, S., Rugh, C. L., Summers, A. O., & Meagher, R. B. (1999). Phytoremediation of methylmercury pollution: MerB expression in Arabidopsis thaliana confers resistance to organomercurials. Proc. Natl. Acad. Sci. USA 96, 6808-6813.

Meagher, R. B. & Rugh, C. L. (1996). Phytoremediation of heavy metal pollution: Ionic and methylmercury. OECD Biotechnology for Water Use and Conservation Workshop. Organization for Economic Co-Operation and Development. Cocoyoc, Mexico. 305-321.

Meagher, R.B., Rugh, C. L., Kandasamy, M. K., Gragson, G., & Wang, N. -J. (1998). Engineered phytoremediation of mercury pollution in soil and water using bacterial genes. Ishndar, I. K., Hardy, S. E., Chang, A. C., & Pierzynski, G. M. Fourth International Conference on the Biogeochemistry of Trace Elements pp. Ann Arbor Press, Inc. Berkeley, CA. 203-221.

Rugh, C. L., et. al. (1996). Mercuric ion reduction and resistance in transgenic Arabidopsis thaliana plants expressing a modified bacterial merA gene. Proc. Natl. Acad. Sci. USA 93, 3182-3187.

Project: 73843 (Renewal of Project No. 55118)

Title: Mechanisms of Heavy Metal Sequestration in Soils: Plant-Microbe Interactions and Organic Matter Aging

PI: Dr. Teresa W. M. Fan *Institution:* University of California at Davis

Publication Type: Journal

Fan, T. W. -M., Pedler, J., Lane, A. N., Crowley, D., & Higashi, R. M. (1997). Comprehensive analysis of organic ligands in whole root exudates using NMR and GC-MS. Analytical Biochemistry. 251, 57-68.

Higashi, R. M., Fan, T. W. -M., & Lan, A. N. (1998). Association of desferrioxamine with humic substances and their interaction with cadmium(II) as studied by pyrolysis gas chromatography mass spectrometry and nuclear magnetic resonance spectroscopy. Analyst. 123(5), 911-918.

Publication Type: Other

Fan, T. W. -M. & Lane, A. N. (1999, in press). NMR in the plant-soil environment. In Encyclopedia of NMR Spectroscopy, John Wiley and Sons, New York, NY.

Fan, T. W. -M. (1996). Recent advancement in profiling plant metabolites by multi-nuclear and multi-dimensional NMR. Shachar-Hill, Y., & Pfeffer, P. E. (Eds.), Nuclear Magnetic Resonance in Plant Biology. American Society of Plant Physiologists. Rockville, MD. 181-254.

Publication Type: Presentation

Fan, T. W. -M., Higashi, R. M., & Crowley, D. E. (1998, Jul.). Plant rhizosphere effects on metal mobilization and transport. DOE EMSP Symposium. Chicago, IL.

Fan, T. W. -M., Shenker, M., Higashi, R. M., Crowley, D. E., & Lane, A. N. (1999, Mar.). Rhizosphere mobilization of heavy metals via plant root exudation. Semi-Annual Meeting of American Chemical Society, Anaheim, CA.

Fan, T. W. -M., Shenker, M., Lane, A. N., Crowley, D., & Higashi, R. M. (1998, Apr.). Comprehensive determination of root exudates under combined Fe deficiency/CD stress by NMR and GC-MS. Society of Environmental Toxicology and Chemistry-Europe. Bordeaux, France.

Fan, T. W. M., Lane, A. N., & Higashi, R. M. (1999, Aug. 22). Structure analysis of soil humates by liquid-state, multinuclear, and multidimensional NMR. Abstr. Pap. Am. Chem. S. 218, U649-U649, Part 1.

Higashi, R. M. & Fan, T. W. -M. (1998, May). Ternary interactions of Cd(II), ligands, and humic substances - implications for metal ion bioavailability. EPA, DOE, ONR, & NSF Joint Workshop.

Higashi, R., Fan, T., Baraud, F., & Lane, A. (1999, Mar.). Ternary interactions of biogenic ligands and Cd(II) with humic substances, with implications for metal ion bioavailability. Semi-annual meeting of the American Chemical Society, Anaheim, CA.

Project: 73858 (Renewal of Project No. 54889)

Title: Chlorinated Hydrocarbon Degradation in Plants: Mechanisms and Enhancement of Phytoremediation of Groundwater Contamination

PI: Dr. Stuart E. Strand *Institution:* University of Washington

Publication Type: Proceeding

Doty, S. L., et. al. (2000). Enhanced metabolism of halogenated hydrocarbons in transgenic plants containing mammalian cytochrome P450 2E1. Proc. National Academy of Sciences. 97, 6287-6291.

Separations Chemistry

Project: 54122

Title: A Broad Spectrum Catalytic System for Removal of Toxic Organics from Water By Deep Oxidation

PI: Dr. Ayusman Sen *Institution:* Pennsylvania State University

Publication Type: Journal

Chlistunoff, J. B. & Johnston, K. P. (1999). UV-Vis spectroscopic determination of the dissociation constant of bichromate from 160°C to 400°C. Journal of Phys. Chem. B. 102, 3993-4003.

Hogan, T., Simpson, R., Lin, M., & Sen, A. (1996). A broad spectrum catalytic system for removal of toxic organics from water by deep oxidation using dioxygen as the oxidant. Catal. Lett. 40, 95.

Hogan, T., Simpson, R., Lin, M., Sen, A. (1997). The deep oxidation of chemical warfare agent models: Facile catalytic oxidative cleavage of phosphorus-carbon and sulfur-carbon bonds using dioxygen. Catal. Lett. 49, 59.

Pifer, A. & Sen, A. (1998). Chemical recycling of plastics to useful organics by oxidative degradation. Agnew. Chem. Int. Ed. 37, 3306.

Pifer, A., et. al. (1999). A broad spectrum catalytic system for the deep oxidation of toxic organics in aqueous medium using dioxygen as the oxidant. J. Am. Chem. Soc. 121, 7485.

Project: 54926

Title: Novel Ceramic-Polymer Composite Membranes for the Separation of Hazardous Liquid Waste

PI: Dr. Yoram Cohen *Institution:* University of California at Los Angeles

Publication Type: Journal

Castro, R. P., Monbouquette, H. G., & Cohen, Y. (1996). Polyvinylpyrrolidone-silica membranes for the treatment of oil-in-water emulsions. J. Membrane Science. 115, 179-187.

Faibish, R., Elimelech, M., & Cohen, Y. (1998). Effect of intraparticle electrostatic double layer interactions on permeate flux decline in crossflow membrane filtration of colloidal suspensions: An experimental investigation. J. Colloid and Interface Science. 204, 77-86.

Jou, J. -D., Yoshida, W., & Cohen, Y. (1999, Sep. 1). A novel ceramic-supported polymer membrane for pervaporation of dilute volatile organic compounds. J. Membrane Sci. 162(1-2), 269-284.

Publication Type: Other

Cohen, Y., Deng-Jeng, J., Yoshida, W., & Bei, N. (1999, in press). Surface modification of oxide surfaces by graft polymerization. Wingrave, J. A. (Ed.). Oxide Surfaces. Marcel Dekker.

Cohen, Y., Faibish, R., & Rovira, M. (1999). Size exclusion chromatography with graft polymerized silica resins. Pefferkorn, E. (Ed.). Surface Interactions in Size Exclusion Chromatography. Marcel Dekker.

Publication Type: Poster

Cohen, Y., Yoshida, W., & Jou, J. -D. (1998, Jul. 27-30). CSP membranes. Invited poster presentation at the DOE First Annual Environmental Management Science Program Scientific Workshop. Rosemont, IL.

Publication Type: Presentation

Cohen, Y. & Jou, J. -D. (1998, May 19-20). Ceramic-supported polymer pervaporation membranes for VOC removal. 10th Annual Meeting of the North American Membrane Society. Cleveland, OH.

Cohen, Y. (1997, Jul.). Graft polymerized ceramic membranes. Gordon Research Conference on Membrane: Materials and Synthesis. New Hampshire.

Cohen, Y. (1998, Sep. 16-17). Polymeric resins for VOC removal from aqueous systems. Volatile Organic Compounds (VOC) Recovery Seminar, EPA/625/R-99/005, ORD, EPA National Risk Management Research Laboratory.

Cohen, Y. (1999, Feb. 9). Polymer surfaces for selective separations. Invited seminar at the DOE Enviromental Molecular Surface Laboratory.

Cohen, Y. (1999, Oct. 31 - Nov. 5). Environmental multimedia distributions of toxics (mend-tox). 1999 AIChE Annual Meeting. Dallas, TX.

Cohen, Y. (2000, Jan. 29 - Feb. 2). Polymer at solid surfaces for novel membranes. Invited presentation at the Chemistry for a Cleaner Environment Conference. Santa Fe, NM.

Cohen, Y., Castro, R. P., Jou, J. -D., & Monbouquette, H. G. (1996, Nov. 10-15). Ceramic-supported polymer membranes for ultrafiltration. AIChE Annual Meeting. Chicago, IL.

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