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Report to Congress on the U.S. Department of Energy's Environmental Management Science Program

Research Funded and Its Linkages to Environmental Cleanup Problems

Environmental Management Science Program Research Award Abstracts

Volume II of III
Appendix B

April 1998

U.S. Department of Energy
Office of Science and Technology
Office of Environmental Management

DISCLAIMER

Appendix B Table of Contents

Environmental Management Science Program Research in:

Introduction

The Department of Energy's Environmental Management Science Program (EMSP) serves as a catalyst for the application of scientific discoveries to the development and deployment of technologies that will lead to reduction of the costs and risks associated with cleaning up the nation's nuclear complex. Appendix B provides details about each of the 202 research awards funded by the EMSP.

This information may prove useful to researchers who are attempting to address the Department's environmental management challenges in their work, program managers who are planning, integrating, and prioritizing Environmental Management projects, and stakeholders and regulators who are interested in the Department's environmental challenges.

The research award information is organized by the state and institution in which the lead principal investigator is located. In many cases, the lead principal investigator is one of several investigators at a number of different institutions. In these cases, the lead investigator (major collaborator) at each of the additional institutions is listed.

Each research award abstract is followed by a list of high cost projects that can potentially be impacted by the research results. High cost projects are Environmental Management projects that have total costs greater than $50 million from the year 2007 and beyond, based on the March 1998 *Accelerating Cleanup: Paths to Closure Draft* data, and have costs or quantities of material associated with an Environmental Management problem area. High cost projects which must remain active in the year 2007 and beyond to manage high risk are also identified. Descriptions of these potentially related high cost Environmental Management projects can be found in Appendix C. Additional projects in the same problem area as a research award can be located using the *Index of High Cost Environmental Management Projects by Problem Area*, at the end of Appendices B and C.

There is no guarantee that the research results will impact the Department's high cost cleanup projects and it is difficult to predict the impact of research results on Departmental cleanup activities. The information presented illustrates some possible ways in which the EMSP can add value to the Department's environmental management cleanup mission by providing the scientific knowledge that could lead to significantly lower cleanup costs and reduced risks to workers, the public, and the environment.

Guide to Fields on Research Award Descriptions

Field Name	Description of Contents
Institution	University, National Laboratory, company, or organization leading the research
Award Number and Title	Research award number and title of research
Year of Award	Fiscal Year in which the research was funded
Amount of Award	Total funding awarded for the life of the research project
Problem Area	Environmental management problem area most closely associated with the research
Science Category/Subcategory	Scientific discipline or category and sub-category with which the research is most closely associated
Principal Investigator	Lead researcher or institutional contact name, e-mail and phone number
Major Collaborator	Additional researchers at other institutions
For More Information	Web site address for more information on the research award
Description Provided by Investigator	Information about the problem the research is to address. This information has been provided by the principal investigator.

Environmental Management Science Program Research in Alabama

Alabama A&M University

55014-AL - Kinetics and Mechanisms of Metal Retention/Release in Geochemical Processes in Soil

Year of Award: 1996 **Amount of Award:** $361,788
Problem Area: Remedial Action
Science Category/SubCategory: Geochemistry / Sorption/Desorption
Principal Investigator: Dr. Robert W. Taylor, 205-851-5462
For More Information: http://www.doe.gov/em52/55014.html

Description Provided by Investigator:

Remediation of soils polluted with heavy metals is a major challenge facing our nation. This is especially so at many DOE facilities and other superfund sites. In many cases, speciation of the metals is inaccurate and difficult and the mechanisms by which the metals are retained/released in soils over long times are poorly understood. Consequently, the long-term fate of metals in soils cannot be precisely predicted and often, the remediation recommendations and techniques that are employed to clean up soils may be ineffective or unnecessary. Accordingly, we are proposing work to generate basic knowledge on the kinetics and mechanism(s) of heavy metal retention/release by soil mineral colloids as affected by inorganic anion. The nature of the interaction of Cd(II), Co(II), Cr(VI), Cu(II), Ni(II) and Pb(II) with pure soil minerals and extracted soil clays will be investigated. The colloids will be characterized in terms of surface area, surface charge and surface site density. They will be used to study the effect(s) of pH, phosphate rate, and temperature on metals retention/release. The experiments will involve using various kinetic and isothermic sorption equations as models to describe the data thus acquired. The spectroscopic methods will involve using extended x-ray absorption fine structure spectroscopy (EXAFS) and Fourier Transform Infrared Spectroscopy (FTIR). The data generated from the proposed study will assist in designing better remediation strategies to effectively clean up toxic heavy metal contaminated soils at DOE facilities and other superfund sites.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ AL007	C-7	Environmental Restoration
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV212	C-49	Underground Test Area (UGTA)
§ NV214	C-53	Industrial Sites
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ OR-48101	C-99	Offsite Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
SR-HL03	C-257	Waste Removal Operations and Tank Closure

Environmental Management Science Program Research in Alabama

University of Alabama

55164-AL - Advanced Experimental Analysis of Controls on Microbial Fe(III) Oxide Reduction

Year of Award: 1996 **Amount of Award:** $427,399
Problem Area: Remedial Action
Science Category/SubCategory: Biogeochemistry / Biogeochemistry
Principal Investigator: Dr. Eric E. Roden, 205-348-0556, eroden@biology.as.ua.edu
For More Information: http://www.doe.gov/em52/55164.html

Description Provided by Investigator:

Fe(III) oxides are ubiquitous components of soils, sediments, and subsurface materials, and are one of the most important sorbents for heavy metals, radionuclides, organic contaminants and organic/metal co-contaminants in the subsurface. These compounds can serve as electron sink for microbial metabolism in anaerobic sedimentary environments, which include portions of many groundwater aquifers removed in space and time from a source of O_2. Recent studies indicate that direct microbial (i.e., enzymatic) catalysis is responsible for most of the Fe(III) oxide reduction occurring in anaerobic soils and sediments, and that Fe(III) oxide reducing bacteria dominate microbial metabolism in environments where Fe(III) oxides are abundant because of their ability to outcompete sulfate-reducing and methanogenic bacteria for common substrates (e.g. acetate and H_2) for anaerobic respiration.

Microbial Fe(III) oxide reduction can have several very important influences on the persistence and mobility of metal/organic contaminants in subsurface environments. It is well-known that metal oxide reduction can cause mobilization of adsorbed metals and radionuclides, and this "reductive dissolution" mechanism is often invoked as an explanation for the release of soluble trace elements in anaerobic sediments and groundwater aquifers. In contrast, production of bicarbonate and hydroxyl alkalinity during Fe(III) oxide reduction may in some cases lead to precipitation of carbonate minerals which can incorporate and thereby immobilize radionuclide and other contaminant metals. In addition, dissolved Fe(II) produced during Fe(III) reduction may displace radionuclides from organic complexants, thereby potentially retarding their mobility in the subsurface. Solid-phase Fe(II) may create considerable surface sorption sites, and may catalyze secondary redox reactions such as reduction of nitrobenzene compounds or reductive dechlorination of carbon tetrachloride. Fe(III) oxide-reducing bacteria (FeRB) can dechlorinate carbon tetrachloride directly, as well as oxidize a variety of chlorinated and non-chlorinated aromatic hydrocarbons of significance in DOE waste streams. These organisms can also reduce metals which are soluble in their oxidized form (e.g. U(VI), Cr(IV)) to an insoluble reduced form, thereby limiting their mobility in the subsurface. They can also reduce Co(III)-EDTA to Co(II)-EDTA, which is likely to be considerably less stable and mobile than Co(III)-EDTA in the subsurface. Fe(II) can also serve as an indirect reductant for Cr (VI) and Co(III).

Considering the broad influence that microbial Fe(III) oxide reduction can have on subsurface metal/organic contaminant biogeochemistry, understanding mechanisms which control this process is critical for predicting the behavior and fate of these contaminants in anaerobic subsurface environments. Perpetuation of many of the processes listed above in subsurface environments will depend on the maintenance of active metal-reducing bacterial populations. Knowledge of factors which influence the rates of growth and activity of Fe(III) oxide-reducing bacteria is thus critical for predicting (i.e. modeling) the long-term influence of these organisms on the fate of contaminants in the subsurface, and for effectively utilizing Fe(III) oxide reduction and associated geochemical affects for the purpose of subsurface metal/organic contaminant bioremediation. Recent DOE Subsurface Science Program-funded research indicates that the surface properties of Fe(III) oxides as well as the surface-chemical properties and nutritional/growth status of Fe(III)-reducing bacteria are critical determinants of the rate and extent of Fe(III) oxide reduction. However, to date laboratory studies of factors controlling the rate and extent of microbial Fe(III) oxide reduction have been conducted mainly in closed-system batch cultures. In contrast, the subsurface represents an open system in which removal of reaction end-products can occur, and in which the kinetics of important precipitation and/or surface complexation reactions may differ substantially from those occurring in closed systems. This research project will refine existing models of microbiological and geochemical controls on Fe(III) oxide reduction, using laboratory reactor systems which mimic to varying degrees the physical and chemical conditions of the subsurface. Novel experimental methods for studying the kinetics of microbial Fe(III) oxide reduction and measuring growth rates of Fe(III) oxide-reducing bacteria will be developed. These new methodologies will be directly applicable to studies of subsurface contaminant transformations directly coupled to or influenced by microbial Fe(III) oxide reduction.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

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Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§ RL-ER08	C-147	Groundwater Management
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Arizona

Northern Arizona University

54898-AZ - Molecular Dissection of the Cellular Mechanisms Involved in Nickel Hyperaccumulation in Plants

Year of Award: 1996 **Amount of Award:** $495,938
Problem Area: Remedial Action
Science Category/SubCategory: Plant Science / Plant Membrane Transport
Principal Investigator: Dr. David Salt, 520-523-3008, David.Salt@nau.edu
For More Information: http://www.doe.gov/em52/54898.html

Description Provided by Investigator:

Phytoremediation, the use of plants for environmental cleanup of pollutants, including toxic metals, holds the potential to allow the economic restoration of heavy metal and radionuclide contaminated sites.

A number of terrestrial plants are known to naturally accumulate high levels of metals in their shoots (1-2 % dry weight), and these plants have been termed metal-hyperaccumulators. Clearly, the genetic traits that determine metal-hyperaccumulation offers the potential for the development of practical phytoremediation processes. Our long-term objective is to rationally design and generate plants ideally suited for phytoremediation using this unique genetic material.

Initially, our strategy will focus on isolating and characterizing the key genetic information needed for expression of the metal-hyperaccumulation phenotype. Recently, histidine has been shown to play a major role in Ni hyperaccumulation. Based on this information we propose to investigate, at the molecular level, the role of histidine biosynthesis in Ni hyperaccumulation in *Thlaspi goesingense,* a Ni hyperaccumulator species.

- We will clone key genes involved in histidine biosynthesis

- We will characterize their transcriptional and post transcriptional regulation by histidine, Ni and other heavy metals, and

- We will determine if any of these genes are essential and sufficient for Ni hyperaccumulation by their expression in the non-hyperaccumulator *Arabidopsis thaliana*

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§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ OR-45301	C-103	Paducah Remedial Action
§+ OR-46301	C-107	Portsmouth Remedial Action
§ RL-ER08	C-147	Groundwater Management
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Arizona

University of Arizona

54908-AZ - Partitioning Tracers for In Situ Detection and Quantification of Dense Nonaqueous Phase Liquids in Groundwater Systems

Year of Award: 1996 **Amount of Award:** $776,903
Problem Area: Remedial Action
Science Category/SubCategory: Hydrogeology / Dense Non-Aqueous Phase Liquid (DNAPL) Dynamics
Principal Investigator: Dr. Mark L. Brusseau, 520-621-1646, brusseau@ag.Arizona.EDU
Major Collaborator(s): Mark White at Pacific Northwest National Laboratory
Mart Oostrom at Pacific Northwest National Laboratory
For More Information: http://www.doe.gov/em52/54908.html

Description Provided by Investigator:

The overall goal of the proposed project is to explore the use of partitioning tracers to characterize dense nonaqueous phase liquids (DNAPLs) in aquifer systems. Bulk-phase partitioning tracers will be investigated to detect and determine DNAPL saturation, while interface partitioning tracers will be investigated to measure the area of the DNAPL-water interface. The specific objectives that will be addressed to accomplish this goal are:

1. Investigate the use of partitioning tracers to detect and determine both the saturation and interfacial area of DNAPLs in saturated porous media.
2. Investigate the effect of rate-limited mass transfer on the transport behavior of partitioning tracers.
3. Investigate the effect of porous-media heterogeneity on the transport behavior of partitioning tracers.
4. Develop and evaluate mathematical models capable of simulating the transport of partitioning tracers in complex systems.

APPROACH

This proposal outlines an integrated approach for the development and testing of a unique method for detecting and measuring DNAPL in aquifer systems. The approach combines one-dimensional laboratory experiments, three-dimensional intermediate-scale flow cell experiments, physical methods for DNAPL description (including dual-energy gamma radiation), and advanced modeling techniques. This approach will allow a new, promising technique for characterizing DNAPL in aquifer systems to be verified by established laboratory and numerical methods. The effect of heterogeneity will be examined by the use of a flow-cell packed with layers of variable permeability and containing multiple sample ports. The effect of rate-limited liquid-liquid mass transfer will be investigated by examining the impact of pore-water velocity and DNAPL form on transport of the partitioning tracers.

EXPECTED RESULTS

Effective risk assessment and remediation of DNAPL contaminated sites is constrained by the limitations of current site characterization techniques. A major weakness of the current methods is that they provide data at discrete points, such that the probability of sampling a zone of localized DNAPL is quite small. The results of the research will lead to improved techniques for characterizing DNAPL contaminated sites and will enhance our understanding of the distribution of DNAPLs in the subsurface. The use of this method will reduce the uncertainty associated with risk assessments and remediation planning.

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Project ID	Page #	Project Title
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Arizona

University of Arizona

59827-AZ - The Influence of Radiation and Multivalent Cation Additions on Phase Separation and Crystallization of Glass

Year of Award: 1997 **Amount of Award:** $723,000
Problem Area: High Level Waste
Science Category/SubCategory: Materials Science / Radiation Effects On Storage Materials
Principal Investigator: Dr. Michael C. Weinberg, 520-621-6909, MCW@U.arizona.edu
For More Information: http://www.doe.gov/em52/59827.html

Description Provided by Investigator:

Recent reviews which have dealt with critical issues regarding the suitability of glasses for nuclear waste disposal have identified liquid-liquid immiscibility and crystallization processes as having the potential to alter significantly storage behavior, especially chemical corrosion characteristics. These phase transformation processes can be abetted (or deterred) by radiation or the inclusion of small quantities of other components such as transition metals, rare earths, actinides, etc. Consequently, in order to minimize the chances for the occurrence of deleterious phase separation or crystallization, it is essential to examine the influence of these factors on phase transformation kinetics.

Although phase separation and crystallization have been studied experimentally in a number of actual and potential waste disposal glasses, little information is available regarding the influence of radiation on such processes. Exposure to radiation causes structural damage in the glass, which can in turn alter the thermodynamic state of glass and/or influence the kinetics occurring in glass. For example, it is not known if radiation damage is likely to alter the mass transport rate sufficiently to affect the region of stability or to produce local changes on the thermodynamics of immiscibility and crystallization.

Thus, the major goal of our program will be to study the influence of irradiation and multivalent cations and redox conditions upon the thermodynamics and kinetics of phase separation and crystallization in selected glass compositions. Also, we will relate any observed changes in transformation behavior to structural modifications caused by radiation. Finally, we will develop guidelines to mitigate the deleterious effects of phase separation and crystallization by composition adjustments, based on the development of a database from ongoing and existing measurements and the development of appropriate models.

The characteristics of phase separation will be analyzed, experimentally, using SEM, EDS, HSEM, TEM, and SAXS. Crystallization will be studied using XRD, SEM, TEM, and optical microscopy. Structural changes will be examined using IR and Raman Spectroscopies and solid state NMR measurements.

The γ irradiation will be performed at PNNL at the Gamma Irradiation Facility located at the Hanford site. The α particle bombardment will be performed at the University of Arizona Physics Department facility and the β-particle bombardment will be performed at the TEM facility at the Arizona Materials Laboratory.

The results of the study will provide fundamental insights into the influence of radiation and multivalent cations on phase transformation processes in glass. By correlating changes in phase separation and crystallization behavior with observed modifications of structure and bonding and by performing modeling we will be able to understand the changes in phase transformation behavior from a basic, mechanistic viewpoint.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§ ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ RL-TW08	C-185	Process Waste Privatization Infrastructure
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§ SR-HL05	C-265	Vitrification
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in Arizona

University of Arizona

60326-AZ - Isolation of Metals from Liquid Wastes: Reactive Scavenging in Turbulent Thermal Reactors

Year of Award: 1997 **Amount of Award:** $1,075,000
Problem Area: Mixed Waste
Science Category/SubCategory: Engineering Science / Design, Process and Modeling
Principal Investigator: Dr. Jost O.L. Wendt, 520-621-6050, wendt@bigdog.engr.arizona.edu
Major Collaborator(s): Dr. William P. Linak at Environmental Protection Agency
Dr. Alan R. Kerstein at Sandia National Laboratories - California
Dr. Arne J Pearlstein at the University of Illinois at Urbana-Champaign
For More Information: http://www.doe.gov/em52/60326.html

Description Provided by Investigator:

Metal-bearing liquids constitute a major part of the DOE waste inventory. This waste is extremely varied with respect to metals (radionuclides, heavy metals, transuranics) and other species (e.g., organics). For much of this waste, concentration of metals to reduce the volume requiring special isolation is critical. One potentially suitable technology is **high-temperature reactive capture of volatile metals by readily available collectable particulate sorbents** (kaolinite, bauxite, and limestone) injected downstream of a flame zone. High temperature reaction between metal vapor and sorbent forms environmentally benign products that are water unleachable.

We propose to begin developing the fundamental science base for understanding and evaluating a class of processes applicable to a broad range of aqueous and nonaqueous feedwastes. **We propose a three-pronged experimental and computational approach** building on our previous work in each area. We will:

- investigate kinetics in a laminar-flow reactor in which the simple flow does not confound extraction of kinetic data. *Ex situ* size-segregated particle analysis will provide data on speciation and kinetics. Drop evaporation and trajectories will be studied using *in situ* laser-induced molecular fluorescence.
- build fundamental models of drop dynamics and evaporation, reaction, particle-size evolution, gas-to-particle conversion, etc., that allow data from the laminar flow reactor at Arizona to be used to predict behavior in a larger, turbulent-flow reactor.
- use data (particle-size distribution, *ex situ* size-segregated particle analysis, etc.) From EPA's 82 kW reactor to improve and validate models that will enable rational evaluation of specific processes.

The work will contribute to rational evaluation of high-temperature thermal processes for DOE metal-bearing liquid waste through the ability to predict particle-size distribution, speciation, and size-segregated speciation. Specifically, **we will address critical scientific issues** relating to high-temperature reactive capture of metals from liquid wastes, including

- the chemistry of metal speciation
- the effect of drop-size variation (due to variation in feedwaste properties, such as surface tension) on thermal history of the drop, and the related effects on evaporation, kinetics, and metal speciation,
- the effect of drop size variation on drop trajectory, with special emphasis on large drops that may be-pass or penetrate the flame zone, and contribute to emissions,
- gas-to-particle conversion of metallic species, with special emphasis on the use of reactive sorbents to scavenge metallic vapors as collectable particulate, and
- the effect of operating conditions (temperature, residence time, drop size and injection velocity, turbulence intensity, and feed composition, including the metal, the liquid, and chlorine or sulfur) on the size distributions

of particles formed from drops that have incompletely volatilized, as well as particles that form as a result of gas-to-particle conversion on injected sorbent.

The advantages of high-temperature reactive scavenging are:

- The organic constituents of some metal-bearing liquid wastes must be treated thermally in order to meet TSCA, RCRA, OSHA, and CAA requirements, and the laws of various states.
- No species need be added to complex liquid systems. The importance of this point is highlighted by recent DOE experience with generation of flammable amounts of benzene vapor by radiolysis of an organic complexant (sodium tetraphenylborate) used to precipitate 137Cs at the Savannah River Site.
- Organics already present are destroyed with high efficiency. This is especially attractive with respect to high-level tank waste at the Hanford Site, in which large amounts of citrate, glyoxylate, EDTA, and HEDTA were added to precipitate radionuclides. These organics are important in generation of flammable gas mixtures episodically vented from 25 tanks on Hanford's Flammable Gas Watch List.
- The same basic approach can be used to treat a broad range of liquid wastes, in each case concentrating the metals (regardless of liquid-phase oxidation state or association with chelators or adsorbents) using a collectable sorbent, and destroying any organic species present.
- The general robustness with respect to gross feedwaste composition promises a relatively high degree of tolerance with respect to inevitable variations in the composition of a given metal-bearing feedwaste.

Finally, an important concern in any nuclear waste treatment process is emissions. In that regard, the Army's exemplary program to destroy stockpiled chemical weapons by incineration is instructive. Without incident, more than 1.4 million kg of nerve gas has been destroyed in two TSCA-, RCRA-, OSHA, and CAA permitted incinerators, a contract has been let for a third, and contracts for two more will be let this year. Like the Army's incineration approach for two nerve gasses and two blister agents, high-temperature reactive capture of metals from liquid waste (accompanied by incineration of any organics in the feedwaste) offers the potential for one basic process to treat (with modifications) a range of feedwastes, thus simplifying design and permitting by avoiding *de novo* process development for each waste composition.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

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Project ID	Page #	Project Title
§ ID-WM-107	C-45	Long Term Treatment/Storage/Disposal Operations
§ RL-WM03	C-193	Solid Waste Storage and Disposal
§+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in California

Rockwell International Corporation

55094-CA - Chemical and Ceramic Methods Toward Safe Storage of Actinides Using Monazite

Year of Award: 1996 **Amount of Award:** $1,287,000
Problem Area: Nuclear Materials
Science Category/SubCategory: Materials Science / Chemical and Structural Properties Of Storage Materials
Principal Investigator: Dr. P.E.D. Morgan, 805-373-4273, pemorgan@scimail.risc.rockwell.com
Major Collaborator(s): Dr. Lynn A. Boatner at Oak Ridge National Laboratory
For More Information: http://www.doe.gov/em52/55094.html

Description Provided by Investigator:

The program will address more particularly the section, "Plutonium behavior in mixed matrices - specialized waste forms", with the concept that monazite ceramic will provide the most safe, most secure, geologically tested, very long term, containment for actinides. That monazites are the ideal crystal hosts for containment of actinide or transuranic elements (extremely stable geologically and resistant to radiation damage) is well established. They were proposed a number of years ago as high level nuclear waste forms at Oak Ridge National Laboratory.

Following the deliberations of the Hench Panel in 1984, and the decision to proceed with borosilicate glass as a low level waste, organized research on monazite and other "alternative waste forms" came to an end. As pointed out in a current National Academy of Science Panel report, approximately fifteen years of potential progress in the development of alternative nuclear waste forms were then lost.

We therefore seek to do basic studies of the ceramic nature of monazite utilizing two groups that have a serious previous background in research concerning monazite and radwaste encapsulation. These are complicated fields and, to avoid unnecessary duplication and waste, it should be important to utilize and to extend that already hard won experience.

The group headed by Lynn Boatner at Oak Ridge National Labs has many years of preeminent experience in studying monazite, while that laboratory is, naturally, in a fine position to transfer basic study results to later engineering application.

The group at the Rockwell Science Center, including Alan Harker and Peter Morgan, became well known for its work in the area of ceramic radwaste hosts and contributed considerable basic understanding to the ceramic problems and advantages, particularly pointing out to the community the key role of the grain boundary leaching phenomena (possible glasses, precipitated grain boundary phases, etc.).

The recent discovery by the Rockwell group, including also David Marshall, that monazite provides weak stable interfaces for ceramic matrix composites has stimulated widespread, renewed interest in the properties of monazite as a ceramic.

The main outstanding fundamental research issues facing the use of monazite as a waste form necessitate the development of fundamental understanding of: sintering mechanisms involved in forming high density monazite ceramics; physical and chemical properties of grain boundaries in these ceramics; interactions with impurities and additives used to promote densification; physical properties of polycrystalline monazite ceramics; and the precipitation of monazite phases in an efficient, simple and economical manner. We propose to address these issues to serve as a knowledge base for using monazite as a nuclear waste form.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Nuclear Materials problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Nuclear Materials".

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+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
+ RL-TW08	C-185	Process Waste Privatization Infrastructure
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
+ SR-HL01	C-249	H-Tank Farm
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in California

Scripps Research Institute

55097-CA - Heavy Metal Pumps in Plants

Year of Award: 1996 **Amount of Award:** $325,309
Problem Area: Remedial Action
Science Category/SubCategory: Plant Science / Plant Membrane Transport
Principal Investigator: Dr. Jeffrey F. Harper, 619-554-2862, harper@scripps.edu
For More Information: http://www.doe.gov/em52/55097.html

Description Provided by Investigator:

Plants have been proposed as a bioremediation tool to help remove toxic heavy metals from contaminated land and water. However, little is known about how plants take up heavy metals from the soil and transport them to different parts of the plant. An important long term goal is to understand how heavy metals are transported across the plasma membrane of plant cells. The research is focused on a putative heavy metal uptake pump, AXA2, identified in a model plant, Arabidopsis. AXA2 belongs to a super-family of ion-translocating P-type ATPases and is most similar to a subfamily of pumps which translocate heavy metals such as copper and cadmium. Three specific aims are proposed (1) Determine the ion specificity of the AXA2 pump, (2) Determine how pumping activity is regulated, and (3) Determine if an increased uptake of heavy metals can be achieved by engineering a transgenic plant with a hyperactive pump. The hypothesis being tested is that AXA2 encodes a high affinity uptake pump for copper, with lower affinity for cadmium, zinc and nickel. Fundamental research on heavy metal transporters may eventually permit transgenic plants to be engineered with specific heavy metal uptake systems useful for bioremediation.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

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Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§ RL-ER08	C-147	Groundwater Management
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in California

United States Department of Agriculture

55278-CA - Molecular Genetics of Metal Detoxification: Prospects for Phytoremediation

Year of Award: 1996 **Amount of Award:** $578,389
Problem Area: Remedial Action
Science Category/SubCategory: Plant Science / Plant Genetics
Principal Investigator: Dr. David W. Ow, 510-559-5909, ow@mendel.berkeley.edu
For More Information: http://www.doe.gov/em52/55278.html

Description Provided by Investigator:

Unlike compounds that can be broken down, the remediation of most heavy metals and radionuclides requires physical extraction from contaminated sources. Plants can extract inorganics, but effective phytoextraction requires plants that produce high biomass, grow rapidly and possess high capacity-uptake for the inorganic substance. Either hyperaccumulator plants must be bred for increased growth and biomass or hyperaccumulation traits must be engineered into fast growing, high biomass plants. This latter approach requires fundamental knowledge of the molecular mechanisms in the uptake and storage of inorganics. Much has been learned in recent years on how plants and certain fungi chelate and transport selected heavy metals. This progress has been facilitated by the use of *Schizosaccharomyces pombe* as a model system. The use of a model organism for study permits rapid characterization of the molecular process. As target genes are identified in a model organism, their sequences can be modified for expression in a heterologous host or aid in the search of homologous genes in more complex organisms. Moreover, as plant nutrient uptake is intrinsically linked to the association with rhizospheric fungi, elucidating metal sequestration in this fungus permits additional opportunities for engineering rhizospheric microbes to assist in phytoextraction.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

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§ RL-ER08	C-147	Groundwater Management
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in California

Lawrence Berkeley National Laboratory

54698-CA - Rapid Mass Spectrometric DNA Diagnostics for Assessing Microbial Community Activity During Bioremediation

Year of Award: 1996 **Amount of Award:** $675,000
Problem Area: Remedial Action
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Biomedical Instrumentation
Principal Investigator: Dr. W. Henry Benner, 510-486-7194, WHBenner@lbl.gov
Major Collaborator(s): Jennie Hunter-Cevera at Lawrence Berkeley National Laboratory
For More Information: http://www.doe.gov/em52/54698.html

Description Provided by Investigator:

The use of DNA-based procedures for the detection of biodegrading organisms or genes that code for pollutant-degrading enzymes constitutes a critical technology for following biochemical transformation and substantiating the impact of bioremediation. In previous studies, DNA-based technology has been demonstrated to be a sensitive technique for tracking micro-organism activity at the molecular level. These procedures can be tuned to identify groups of organisms, specific organisms, and to detect signals that measure microbial community activity. This proposal describes the evaluation of a monitoring strategy that relies on the combined use of DNA diagnostics with mass spectrometry as the detection scheme. The intent of this work is a two-fold evaluation of: 1) the feasibility of replacing the use of gel separations for identifying polymerase chain reaction (PCR) products with a rapid and automatable form of electrospray mass spectrometry and 2) the use of matrix-assisted-laser-desorption-ionization mass spectrometry (MALDI-MS) as a tool to score oligonucleotide ligation assays (OLA).

Mass spectrometry is an attractive detection alternative for PCR and OLA procedures because it is a sensitive analytical technique capable of providing high sample throughput performance and the introduction of samples into a mass spectrometer is automatable. Mass spectra are generated rapidly, in the order of minutes, thus eliminating a time bottleneck caused by time-consuming gel electrophoresis separations. The adaptation of OLA for mass spectrometric analysis will cut costs by eliminating expensive reagents. The techniques are automatable which translates into a decreased human error rate when numerous samples are analyzed as a component of large scale bioremediation studies. The successful conclusion of the work will be the development of a mass spectrometry capability for sizing PCR products and scoring OLA tests in formats that provide high throughput and automation for bioremediation studies.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

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§ RL-ER08	C-147	Groundwater Management
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in California

Lawrence Berkeley National Laboratory

55264-CA - Subsurface High Resolution Definition of Subsurface Heterogeneity for Understanding the Biodynamics of Natural Field Systems: Advancing the Ability for Scaling to Field Conditions

Year of Award: 1996 **Amount of Award:** $2,790,455
Problem Area: Remedial Action
Science Category/SubCategory: Microbial Science / Microbial Transport
Principal Investigator: Dr. Ernest L. Majer, 510-486-5875, elm@ccs.lbl.gov
Major Collaborator(s): Dr. Thomas M. Stoops at Idaho National Engineering and Environmental Laboratory
Dr. Fred J. Brockman at Pacific Northwest National Laboratory
For More Information: http://www.doe.gov/em52/55264.html

Description Provided by Investigator:

This research is an integrated physical (geophysical and hydrologic) and microbial study using innovative geophysical imaging and microbial characterization methods to identify key scales of physical heterogeneities that affect the biodynamics of natural subsurface environments. Data from controlled laboratory and in situ experiments at the INEL TAN site will be used to determine the dominant physical characteristics (lithologic, structural, and hydrologic) that can be imaged in situ and correlated with the microbial properties. Emphasis will be placed on identifying fundamental scales of variation of physical parameters that control transport behavior relative to predicting subsurface microbial dynamics. A key hypothesis addressed is that nutrient flux and transport properties are key factors in controlling microbial dynamics. The outcome will be an improved understanding of the relationship between physical and microbial heterogeneity, thus facilitating the design of bioremediation strategies in similar environments. The work described here is an extension of current basic research on natural heterogeneity within the DOE/OHER Subsurface Science Program (SSP) and is intended to be one of the building blocks of an integrated and collaborative approach with an INEL/PNL effort aimed at understanding the effect of physical heterogeneity on transport properties and biodynamics in natural systems.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

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§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§ RL-ER08	C-147	Groundwater Management
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in California

Lawrence Berkeley National Laboratory

55318-CA - Improved Analytical Characterization of Solid Waste-Forms by Fundamental Development of Laser Ablation Technology

Year of Award: 1996 **Amount of Award:** $1,229,167
Problem Area: High Level Waste
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Laser Ablation Techniques
Principal Investigator: Dr. Richard E. Russo, 510-486-4258, RERusso@lbl.gov
For More Information: http://www.doe.gov/em52/55318.html

Description Provided by Investigator:

Chemical characterization is listed as the top priority need in every DOE EM major problem area (high-level waste tanks, contaminant plumes, D&D activities, spent nuclear fuel, mixed wastes, landfills, etc.). The DOE National Laboratories have invested millions of dollars in effort and equipment in order to utilize laser ablation technology to address chemical characterization needs within these problem areas. However, fundamental laser ablation processes are not being addressed in these studies, but rather specific applications of a complex, unknown technology. Laser ablation must be understood on a fundamental level to insure confidence in the characterization for DOE environmental applications.

This proposed EMSP research will address several fundamental issues, including energy coupling, mass removal, gas dynamics, and transport. Energy coupling is critical in that it governs the sensitivity and accuracy of constituent removal. Experiments will provide new knowledge on space charge effects, plasma screening, and plasma expansion. This research plans to investigate calibration technologies that do not rely on "matched" standards. For the diverse mixed-waste samples from DOE environmental sites, standards will not exist and it will not be practical to fabricate them. Solid vapor entrainment and transport processes can significantly influence sensitivity and accuracy and will be investigated. The particle size distribution generated during laser ablation influences transport. Mechanisms responsible for particle generation will be addressed. Samples to be emphasized initially in this fundamental research will include prototypic vitrified waste glass and metal/metal-oxide systems. This fundamental work will support the efforts at all the National Laboratories investigating laser ablation technology for the management of DOE radioactive, hazardous chemical, and mixed waste.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

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Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§+ RL-TW04	C-169	Retrieval Project
§+ RL-TW05	C-173	Process Waste Support
§+ SR-HL01	C-249	H-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
ID-WM-107	C-45	Long Term Treatment/Storage/Disposal Operations
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ OR-45301	C-103	Paducah Remedial Action
RL-ER08	C-147	Groundwater Management
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-WM03	C-193	Solid Waste Storage and Disposal
RL-WM04	C-197	Solid Waste Treatment
+ SR-SW02	C-285	Transuranic Waste Project
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in California

Lawrence Berkeley National Laboratory

55343-CA - Enzyme Engineering for Biodegradation of Chlorinated Organic Pollutants

Year of Award: 1996 **Amount of Award:** $550,000
Problem Area: Remedial Action
Science Category/SubCategory: Health Science / Molecular, Structural and Genomic Science
Principal Investigator: Dr. Peter G. Schultz, 510-486-4999, WONGK@UCLINK4.BERKELEY.EDU
For More Information: http://www.doe.gov/em52/55343.html

Description Provided by Investigator:

Halogenated organic compounds have had widespread use as fungicides, herbicides, insecticides, algaecides, plasticizers, solvents, hydraulic fluids, refrigerants and intermediates for chemical syntheses. As a result, they constitute one of the largest groups of environmental pollutants. Chlorinated organic compounds comprise the largest fraction of these materials, having been synthesized by large scale processes over the past few decades. Their ubiquitous use and distribution in our ecosystem has raised concern over their possible effects on public health and the environment.

The biodegradation potential of halogenated compounds is difficult and not well understood. Biological cleavage of carbon-halide bonds can be achieved by either enzymatic or biocatalytic dehalogenation or by spontaneous chemical dehalogenation of unstable intermediates. This research involves the protein engineering of existing enzymes and the "creation" of new enzymes (catalytic antibodies) with enhanced dechlorination capability for a wide variety of chlorinated organic pollutants. These enzymes could be used as such or could be inserted into microorganisms designed for high activity in contaminated environments.

Development of antibodies that catalyze the hydrolysis of halogenated aromatics will be carried out through a combination of chemical and genetic approaches. Haptens will be developed to generate antibodies that stabilize the transition state for hydrolysis of halogenated nitroaromatics. We will then randomize the variable regions of the antibodies and screen for antibodies with enhanced catalytic properties. If successful such an approach could be generalized and might allow one to tailor the specificity of a bioremediation catalyst for a given synthetic halogenated aromatic using the machinery of the immune system.

We will also attempt to clone, express, purify and to determine the structure and chemical mechanism of a known detoxifying enzyme, dechlorinating dehalogenase. In addition, knowledge gained from such studies will be used to redesign the dehalogenase for the purpose of expanding its biodegradative potential to include environmental pollutants that are currently non-biodegradable.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

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§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§ RL-ER08	C-147	Groundwater Management
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in California

Lawrence Berkeley National Laboratory

55351-CA - Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL

Year of Award: 1996 **Amount of Award:** $762,508
Problem Area: Remedial Action
Science Category/SubCategory: Geochemistry / Colloidal Chemistry and Transport
Principal Investigator: Dr. Donald J. DePaolo, 510-486-5875, depaolo@socrates.berkeley.edu
Major Collaborator(s): B. Mack Kennedy at Lawrence Berkeley National Laboratory
For More Information: http://www.doe.gov/em52/55351.html

Description Provided by Investigator:

The research will explore and refine the use of isotopic ratio measurements on aquifer groundwaters and vadose zone gas for improving remediation strategies and increasing the efficiency of ongoing remediation activities at the TAN and RWMC (SDA) sites at Idaho National Engineering Laboratory. The measurements to be made are ∂^{13}C, Δ^{14}C, ∂^{18}O, ∂D, ^{87}Sr/^{86} Sr, and ^{37}Cl/^{35}Cl isotopic ratios, and the abundances and isotopic compositions of the noble gases He, Ne, Ar and Xe.

The isotopic ratios are used in conjunction with water and gas chemistry to determine: (1) the extent and nature of chemical reactions in the TAN plume and their role in retardation of radioactive isotopes ^{90}Sr and ^{137}Cs and the attenuation of dissolved chlorinated hydrocarbons; (2) predict the chemical effects of proposed remediation techniques (bioremediation, oxidation, and grout barrier installation) on transport in the plume; (3) the extent of natural degradation of chlorinated hydrocarbons in the TAN plume, and the transport of gases through the vadose zone from the plume; (4) the extent of natural remediation and in situ transformations of volatile organic compounds at the SDA site; (5) the extent of recirculation of surface air during VVE activities, and how this changes with season and barometric conditions. The data collected will provide a unique characterization of transport processes in the aquifer and the vadose zone, and an evaluation of the benefits of isotopic approaches in support of remediation activities at two representative sites.

The proposed studies are to be carried out in cooperation with the LITCO-supervised characterization and remediation activities at the TAN and RWMC (SDA) sites at INEL. Most of the sampling necessary for the study is covered by normal sampling schedules; additional sampling can be done in existing wells or with soil gas sampling equipment.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

Environmental Management Science Program Research in California

Lawrence Berkeley National Laboratory

55356-CA - Environmentally-induced Malignancies: An In Vivo Model to Evaluate the Health Impact of Chemicals in Mixed Waste

Year of Award: 1996 **Amount of Award:** $969,987
Problem Area: Health / Ecology / Risk
Science Category/SubCategory: Health Science / Health Effects
Principal Investigator: Dr. Maria Pallavicini, 510-486-6124, MGPallavicini@lbl.gov
For More Information: http://www.doe.gov/em52/55356.html

Description Provided by Investigator:

Increased rates of malignancy following exposure to genotoxic agents in the environment are a major public concern. The long term health effects of exposure to complex mixtures of chemicals and radionuclides are of particular concern because their biologic effects may increase risk of malignancy. Multiple genetic alterations reflecting genomic instability and inactivation of cell cycle checkpoints accumulate in malignant cells. Our data suggest that accumulation of genetic changes in hsc occurs during leukemic progression. Hsc, normally quiescent, are recruited into cycle following hemotoxic insult, which facilitates generation of progeny with altered genomes. Chemicals that increase the rate of genomic instability in hsc are likely to increase the frequency of hsc with altered genomes. We predict that complex mixtures of chemicals with leukemogenic potential will 1) be hemotoxic and thus trigger hsc into cycle, and 2) induce genomic instability in hsc. We also predict that chronic low dose exposures to genotoxins with concomitant hemotoxicity will increase the number of cycling hsc and elevate the risk of leukemogenesis by providing more opportunities to "fix" genetic damage in hsc. Mixed waste containing chemicals that are hemotoxic and genotoxic may be associated with a higher risk of leukemogenesis than exposure to either compound alone. We will use molecular and cellular approaches and animal models to establish the relationship between hemotoxicity, genomic instability and genetically aberrant hsc in mice exposed to radiation, benzene and trichloroethylene. Data generated in this project will a) lend insight into mechanisms underlying environmental-induction of leukemic progression, b) facilitate development of a rationale to identify chemical combinations that increase or decrease leukemogenic potential and c) provide opportunities to optimize approaches for biomonitoring and risk assessment.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Health / Ecology / Risk problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Health / Ecology / Risk".

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Project ID	Page #	Project Title
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation

Environmental Management Science Program Research in California

Lawrence Berkeley National Laboratory

55359-CA - Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone

Year of Award: 1996 **Amount of Award:** $1,440,000
Problem Area: Remedial Action
Science Category/SubCategory: Hydrogeology / Instrumentation and Modelling
Principal Investigator: Dr. Boris Faybishenko, 510-486-4852, bfayb@lbl.gov
For More Information: http://www.doe.gov/em52/55359.html

Description Provided by Investigator:

Understanding subsurface flow and transport processes is critical for effective assessment, decision-making, and remediation activities for contaminated sites. However, for fluid flow and contaminant transport through fractured vadose zones, traditional hydrogeological approaches are often found to be inadequate. In this project, we will examine flow and transport through a fractured vadose zone as a deterministic chaotic dynamical process, and develop a model of it in these terms. We will first examine separately the geometric model of fractured rock and the flow dynamics model needed to describe chaotic behavior, then put the geometry and flow dynamics together to develop a chaotic-dynamical model of flow and transport in a fractured vadose zone. We will use the model to predict the long-term bounds on fluid flow and transport behavior, known as the attractor of the system, and examine the limits of short-term predictability within these bounds. This approach is especially well-suited to the need for short-term predictions to support remediation decisions, and long-term bounding studies. We will conduct laboratory and field experiments designed to test the model. In the field experiments, we will measure the timevariation of water flux, moisture content, and hydraulic head at various locations, as well as the total inflow rate to the subsurface. Such variations reflect the changes in the geometry and physics of water flow that display chaotic behavior, which we will try to reconstruct using the data obtained.

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Project ID	Page #	Project Title
§ NV212	C-49	Underground Test Area (UGTA)

Environmental Management Science Program Research in California

Lawrence Berkeley National Laboratory

55396-CA - Sorption of Colloids, Organics, and Metals onto Gas-Water Interfaces: Transport Mechanisms and Potential Remediation Technology

Year of Award: 1996 **Amount of Award:** $1,387,356
Problem Area: Remedial Action
Science Category/SubCategory: Geochemistry / Sorption/Desorption
Principal Investigator: Dr. Jiamin Wan, 510-486-6004, jwan@Csa2.LBL.Gov
For More Information: http://www.doe.gov/em52/55396.html

Description Provided by Investigator:

Although the process of contaminant sorption at mineral surfaces has received much recognition as a major mechanism controlling contaminant behavior in subsurface environments, virtually no attention has been given to the possibility of contaminant sorption at gas-water interfaces. Moreover, no effort has yet been advanced to optimize such interactions for the purpose of facilitating in-situ remediation. Gas-water interfaces, unlike water-solid interfaces, are mobile. Therefore, associations of contaminants with gas-water interfaces can be very important not only in subsurface contaminant distributions, but also in contaminant mobilization, and potentially in remediation.

The first objective of this research is to develop a fundamental understanding of interactions between contaminants and gas-water interfaces, with emphasis on sorption behavior of mixed contaminant systems. We hypothesize that hydrophobic organic contaminants, and natural organic matter can sorb onto the gas-water interfaces, thereby altering interfacial hydrophobicity, and permitting sorption of colloids, metals, and radionuclides onto the gas-water interfaces. This hypothesis will be tested through two tasks: 1. quantifying sorption of individual contaminants at static and dynamic gas-water interfaces, and 2. quantifying sorption of contaminant mixtures at static and dynamic gas-water interfaces. Contaminants to be tested will include TCE, toluene, Pb^{2+}, CrO_4^{2-}, Cs^+, and Sr^{2+}. Inorganic colloids included in this study are kaolinite, smectite (nontronite), and an iron oxide (goethite).

Quantifying partitioning of the contaminants between static interfacial regions and bulk solutions will based on radiometric methods, synchrotron x-ray fluorescence microprobe, and surface tension measurements. In task 1, each contaminant will be tested individually, under a range of solution chemistries (pH 4 to 9, ionic strength 1 to 100 mM). In task 2, different combinations of contaminants (co-contaminants) will be tested. Comparing these results, we expect to significantly improve the understanding of how single and mixed contaminants partition at gas-water interfaces.

The combined results from experiments on static and dynamic gas-water interfaces provide insights into carrying capacities and interfacial contaminant transport. The overall results will provide, for the first time, a useful data base on the poorly understood phenomenon of contaminant interactions with the gas-water interface. These results will improve our current conceptual models of contaminant behavior in subsurface environments.

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Project ID	Page #	Project Title
§ AL024	C-3	Grand Junction Office (GJO) All Other Projects
§ AL007	C-7	Environmental Restoration
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV214	C-53	Industrial Sites
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ OR-48101	C-99	Offsite Remedial Action
§+ OR-45301	C-103	Paducah Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ RF014	C-213	Industrial Zone Closure Project
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in California

Lawrence Berkeley National Laboratory

60296-CA - Research Program to Investigate the Fundamental Chemistry of Technetium

Year of Award: 1997 **Amount of Award:** $900,000
Problem Area: High Level Waste
Science Category/SubCategory: Inorganic Chemistry / Solid/Solution Chemistry
Principal Investigator: Dr. Norman M. Edelstein, 510-486-5624, nedel@lbl.gov
Major Collaborator(s): Dr. Carol J. Burns at Los Alamos National Laboratory
For More Information: http://www.doe.gov/em52/60296.html

Description Provided by Investigator:

Technetium (99Tc half-life = 2.13×10^5 years, β-emitter) has been expected to be found in the aqueous phase of nuclear waste tanks primarily as pertechnetate (TcO_4^-) but recent studies indicate that a significant fraction of the Tc is in a different chemical form. This program addresses the fundamental solution chemistry of technetium in the waste tank environment, and in a second part, the stability of Tc in various waste forms. The solution and solid state chemistry of this element will be studied in aqueous solutions at high pH values, with various salts added such as nitrate and nitrite, and as a function of radiation dose, to determine if radiolysis effects cause the reduction of the TcO_4^-. A separate facet of this research is the search for stable lower valent forms of Tc that may be thermodynamically and/or kinetically stable and may be incorporated in various waste forms for long term storage. This phase of the program will address the problem of the possible oxidation of low solubility lower valent compounds of Tc in various waste form matrices and the subsequent leaching of highly soluble TcO_4^-.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

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Project ID	Page #	Project Title
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations

Environmental Management Science Program Research in California

Lawrence Berkeley National Laboratory

60328-CA - High Frequency Electromagnetic Impedance Measurements for Characterization, Monitoring and Verification Efforts

Year of Award: 1997 **Amount of Award:** $816,000
Problem Area: Remedial Action
Science Category/SubCategory: Geophysics / Subsurface Imaging
Principal Investigator: Dr. Ki Ha Lee, 510-486-7468, KHLee@lbl.gov
For More Information: http://www.doe.gov/em52/60328.html

Description Provided by Investigator:

We propose to develop high-frequency impedance (HFI) methodology utilizing a window of the electromagnetic (em) spectrum from 1.0 MHz to 100 MHz. This window, between GPR and low-frequency induction techniques, has not been used to non-invasively investigate the upper few meters of the ground for environmental applications. Modeling and physical parameter studies confirm that impedance measurements at this frequency band can yield high-resolution mapping of the electrical conductivity as well as the permittivity. It is well known that impedance method is free of source coupling, so that the ensuing analysis tends to be much simpler. The research plan consists of three tasks: 1) development of high frequency field measurement techniques, 2) plane wave impedance estimation, and 3) data processing, analysis, and interpretation. These tasks will be investigated in a three-phase approach, roughly corresponding to three years. The proof-concept will be determined with off-the-shelf test instrumentation and commercially available components, and the theoretical methods for impedance estimation, survey design, and sensitivity analysis will be fully developed, during phase 1. The proof-of-concept will provide the specifications necessary for assembling a prototype system, using off-the-shelf components and a modest engineering effort, in phase 2. Phase 3 will include the development of a data analysis package and field testing of the prototype system in order to verify the concept and proper operational procedures in known, well-characterized environments.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV212	C-49	Underground Test Area (UGTA)
§ NV214	C-53	Industrial Sites
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER02	C-129	200 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ RF014	C-213	Industrial Zone Closure Project
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
ID-HLW-101	C-29	High-Level Waste Pretreatment
+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW04	C-169	Retrieval Project
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
+ SR-HL01	C-249	H-Tank Farm
+ SR-HL02	C-253	F-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations

Environmental Management Science Program Research in California

Lawrence Berkeley National Laboratory

60370-CA - Rational Design of Metal Ion Sequestering Agents

Year of Award: 1997 **Amount of Award:** $405,000
Problem Area: Mixed Waste
Science Category/SubCategory: Actinide Chemistry / Actinide (Heavy Element) Chemistry
Principal Investigator: Dr. Kenneth N. Raymond, 510-486-6145, raymond@socrates.berkeley.edu
For More Information: http://www.doe.gov/em52/60370.html

Description Provided by Investigator:

An enormous amount of radioactive and toxic chemical waste remains at over one hundred sites managed by the Department of Energy. Despite the investment of large sums major goals associated with the cleanup remain unmet. It is our thesis that economically practical accomplishments of these tasks will require technology not yet available. Basic studies of the sequestration of the relevant toxic metal ions is required in order to develop processes that will treat effluents sufficiently well to allow direct release into the environment, and minimize the production of secondary wastes. This research group has for many years led the development of new, metal-ion-selective sequestering agents. In what has been described as the first rational synthesis of such an agent, decontamination for Pu4+ have been developed. What is now proposed is the full thermodynamic and structural characterization of the metal-ligan systems that form the basis for rational metal-ion-specific ligand design. This will provide the basis for technologies targeted towards the separation and immobilization of hazardous metal ions. This project encompasses the synthesis of new materials, the physical characterization and evaluation of those materials, and the evaluation (and subsequent improvement) of these materials for interface to applied separation technologies.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW03	C-287	Mixed Low Level Waste Project
ID-HLW-101	C-29	High-Level Waste Pretreatment
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW04	C-169	Retrieval Project
+ RL-TW05	C-173	Process Waste Support
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project
+ SR-HL01	C-249	H-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations

Environmental Management Science Program Research in California

Lawrence Livermore National Laboratory

54950-CA - Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes

Year of Award: 1996 **Amount of Award:** $1,200,000
Problem Area: Remedial Action
Science Category/SubCategory: Hydrogeology / Instrumentation and Modelling
Principal Investigator: Dr. Charles R. Carrigan, 510-422-3941, carrigan@s94.es.llnl.gov
For More Information: http://www.doe.gov/em52/54950.html

Description Provided by Investigator:

Many releases of chemical solvents or DNAPLS occur at the surface causing the vadose layer to be the first part of a hydrologic system to interact with the contaminant. As the entry point of these chemicals into a groundwater system, the vadose zone can become a long-term source function for contamination that is metered by natural processes into the underlying saturated zone for further dispersal. However, a contaminant plume does not remain unaffected by the surrounding unsaturated soil. Heterogeneous vadose regimes, such as those containing fractures or other permeability heterogeneities, are the sites of complex interactions between the atmosphere and groundwater. When a volatile contaminant exists as free product or in dissolved form in the vadose environment, upward transport can occur with the contaminant ultimately being vented as a vapor into the atmosphere. It is known that partitioning of a liquid contaminant into the vapor phase can be a very effective means of decontamination. The subsequent transport of the vapor occurs naturally and can be enhanced, for example, by the anisotropy resulting from fractured-matrix-flow paths as well as by certain heterogeneity distributions. Several stages in the transport process are involved in going from a volatile, liquid state contaminant to a contaminant vapor vented at the surface. In a three-year effort, we will investigate the detailed nature of each of these stages of transport in the vadose zones of fractured and heterogeneous regimes with the (1) aid of existing data, (2) new field studies involving dissolved tracer gases and (3) 3-D diagnostic computer simulations that provide a framework to interpret our observations. We will emphasize determining the impact of features specific to a site, that is, the local geology and hydrology, on each stage of the transport process. In particular we want to better understand how the time scales for (1) partitioning contaminants from the liquid to the vapor states and then (2) transporting the vapor out of the vadose regime are dependent on the specific character of a site. Such time-scale information will be important for determining the appropriate response to vadose zone contamination including the option of natural remediation, that is, no response. This information can also be interpreted as a baseline performance criterion for proposed soil-venting schemes. Not least, this work will result in the development of new field methods, involving the injection and analysis of dissolved rare-isotope and chemical-compound tracers, that we anticipate applying to sites at Lawrence Livermore and to the thick, fractured basalt vadose regime at the Idaho National Engineering Laboratory.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ NV212	C-49	Underground Test Area (UGTA)

Environmental Management Science Program Research in California

Lawrence Livermore National Laboratory

55011-CA - Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes

Year of Award: 1996 **Amount of Award:** $1,088,135
Problem Area: Remedial Action
Science Category/SubCategory: Geophysics / Subsurface Imaging
Principal Investigator: Dr. James G. Berryman, 510-423-2905, berryman@s123.es.llnl.gov
For More Information: http://www.doe.gov/em52/55011.html

Description Provided by Investigator:

Electromagnetic induction tomography is a promising new tool for imaging electrical conductivity variations in the earth. The EM source field is produced by induction coil (magnetic dipole) transmitters deployed at the surface or in boreholes. Vertical and horizontal component magnetic field detectors are deployed in other boreholes or on the surface. Sources and receivers are typically deployed in a configuration surrounding the region of interest. The goal of this procedure is to image electrical conductivity variations in the earth, much as x-ray tomography is used to image density variations through cross-sections of the body. Although field techniques are being developed rapidly at the present time, the algorithms for inverting the magnetic data to produce the desired images of electrical conductivity have not kept pace. The current state of the art in electromagnetic data inversion uses the Born/Rytov approximation (based on a low contrast assumption), even though it is known that conductivity variations range over several orders of magnitude and therefore require nonlinear analysis. In addition, previous field experiments were conducted at controlled test sites that typically do not have extensive external noise or surface clutter problems often associated with environmental sites. Use of the same field techniques in more typical environments is expected to require a new set of data processing tools to remove the effects of both noise and clutter. This project will join theory and experiment to produce enhanced images of electrically conducting fluids underground, allowing better localization of contaminants and improved planning strategies for the subsequent remediation efforts.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

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"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV212	C-49	Underground Test Area (UGTA)
§ NV214	C-53	Industrial Sites
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER02	C-129	200 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in California

Lawrence Livermore National Laboratory

55148-CA - Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry Measurements

Year of Award: 1996 **Amount of Award:** $1,563,436
Problem Area: Remedial Action
Science Category/SubCategory: Geochemistry / Sorption/Desorption
Principal Investigator: Dr. Gregory Nimz, 510-423-2766, nimz1@llnl.gov
Major Collaborator(s): Marc W. Caffee at the University of California at Santa Cruz
For More Information: http://www.doe.gov/em52/55148.html

Description Provided by Investigator:

We propose to identify and quantify the geochemical parameters controlling the migration of key radionuclides (^{36}Cl, ^{90}Sr, ^{93}Zr, ^{99}Tc, and ^{129}I) in undisturbed soils of the shallow and deep vadose zone. Currently, the scientific understanding of these parameters cannot sufficiently meet the requirements for at least two determinations necessary for environmental management in the United States: moisture flux through unsaturated soils, and contaminant radionuclide migration in the far-field environment. The proposed radionuclide measurements will be made using newly developed techniques employing accelerator mass spectrometry (AMS), which provides the required analytical sensitivity such that this work can be conducted for the first time. The research is composed of five components: (1) developing the AMS analytical methods for ^{90}Sr, ^{93}Zr, and ^{99}Tc, and improving AMS methods for ^{36}Cl and ^{129}I; (2) using ^{36}Cl and elemental chlorine analyses from samples collected from a shallow-zone trench and an existing deep-zone (450 meter) drill core to define moisture flux throughout a thick vadose zone in southern Nevada; (3) measuring the distribution of ^{90}Sr, ^{93}Zr, ^{99}Tc, and ^{129}I relative to the defined moisture flux in the shallow vadose zone (where these nuclides occur due to atmospheric nuclear testing); (4) developing a numerical model based on these data that simulates the transport of these radionuclides using a flow-and-transport computer code previously developed at LLNL; and (5) using this numerical model and the moisture flux information obtained from the deep core to simulate the behavior of ^{90}Sr, ^{93}Zr, ^{99}Tc, and ^{129}I in the deep vadose zone. Our investigations in the shallow-zone, where the relationship between nuclide concentration and soil characteristics (composition, texture) can be identified, are expected to greatly improve our understanding of the relationship between chlorine-^{36}Cl distribution and moisture flux. The work on the deep-zone, and the resulting numerical model, is expected to provide a much clearer understanding of the potential for radionuclide transport far away from the contaminant release point, in an environment that is otherwise natural and undisturbed (i.e., in the far-field environment). The radionuclides targeted in this study were distributed globally during the era of atmospheric nuclear testing, and occur in virtually all geological and biological environments. Our development of ultrasensitive AMS techniques for their detection in small samples will provide the means to assess radionuclide migration in most of these environments. This will result in a far greater understanding of potential health risks in the far-field environment, where the public is most likely to come into contact with contaminants. The targeted radionuclides are not only themselves common contaminants, but also are representative of classes of radionuclides and heavy metals that exhibit similar migration behavior. The models developed in this research will therefore furnish a foundation for a wide variety of contaminant migration assessments.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

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Project ID	Page #	Project Title
§ NV212	C-49	Underground Test Area (UGTA)
SR-HL03	C-257	Waste Removal Operations and Tank Closure

Environmental Management Science Program Research in California

Lawrence Livermore National Laboratory

55249-CA - Experimental Determination of Contaminant Metal Mobility as a Function of Temperature Time and Solution Chemistry

Year of Award: 1996 **Amount of Award:** $1,130,000
Problem Area: Remedial Action
Science Category/SubCategory: Geochemistry / Sorption/Desorption
Principal Investigator: Dr. Susan Carroll, 510-423-5694, CARROLL@S92.ES.LLNL.GOV
Major Collaborator(s): Dr. Peggy O'Day at Arizona State University
For More Information: http://www.doe.gov/em52/55249.html

Description Provided by Investigator:

We propose to determine the geochemical processes that control the mobility of Sr in the presence of clays (kaolinite, montmorillonite) and iron hydroxides (goethite) as a function of temperature, pH, and time. The objective of this work is to determine the fundamental data needed to predict the behavior of Sr at temperature and time scales appropriate to thermal remediation. Our approach combines macroscopic sorption/precipitation and desorption/dissolution kinetic experiments, which track changes in solution composition, with direct molecular characterization of Sr in the solid phase using X-ray absorption spectroscopy. These experiments will be used to identify mechanistic geochemical reactions and their themochemical properties that will be incorporated into geochemical computer codes.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

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"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ AL007	C-7	Environmental Restoration
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV212	C-49	Underground Test Area (UGTA)
§ NV214	C-53	Industrial Sites
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ RF014	C-213	Industrial Zone Closure Project
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
OR-43204	C-77	ORNL Bethel Valley Deactivation and Decommissioning

Environmental Management Science Program Research in California

Lawrence Livermore National Laboratory

55411-CA - Joint Inversion of Geophysical Data for Site Characterization and Restoration Monitoring

Year of Award: 1996 **Amount of Award:** $1,272,420
Problem Area: Remedial Action
Science Category/SubCategory: Geophysics / Subsurface Imaging
Principal Investigator: Dr. Patricia A. Berge, 510-423-4829, berge@s44.es.llnl.gov
Major Collaborator(s): James G. Berryman at Lawrence Livermore National Laboratory
For More Information: http://www.doe.gov/em52/55411.html

Description Provided by Investigator:

Work will be carried out by Principal Investigator (PI) P. A. Berge and co-PIs J. G. Berryman, J.J. Roberts, and M. J. Wilt. Propose to develop a code for joint inversion of seismic and electrical data, to improve underground imaging for site characterization and remediation monitoring. Will invert the geophysical data to obtain direct estimates of porosity and saturation, rather than inverting for seismic velocity and electrical resistivity. In the first year, will perform laboratory measurements of elastic and electrical properties of sand-clay mixtures containing contaminants. Also will develop algorithms relating geophysical properties to porosity and saturation, using rock physics theories, geostatistical and empirical techniques, and available laboratory measurements. In the second year, will test the inversion code on available borehole log data to predict properties of cores. In the third year, will carry out a field experiment and invert the seismic and electrical data using the code.

{berge_image.gif - Joint Inversion of Geophysical Data}

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

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"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ RL-ER02	C-129	200 Area Remedial Action
+ RL-TW04	C-169	Retrieval Project
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
+ SR-HL02	C-253	F-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations

Environmental Management Science Program Research in California

Lawrence Livermore National Laboratory

60319-CA - Thermodynamics of the Volatilization of Actinide Metals in the High-Temperature Treatment of Radioactive Wastes

Year of Award: 1997 **Amount of Award:** $900,000
Problem Area: Nuclear Materials
Science Category/SubCategory: Actinide Chemistry / Actinide (Heavy Element) Chemistry
Principal Investigator: Dr. Martyn G. Adamson, 510-423-2024, adamson1@llnl.gov
Major Collaborator(s): Donald R. Olander at the University of California at Berkeley
For More Information: http://www.doe.gov/em52/60319.html

Description Provided by Investigator:

We are proposing to perform a detailed study of the volatilization behavior of the U, Pu and possibly Am under conditions relevant to the thermal treatment (destruction) of actinide-containing organic-based mixed and radioactive wastes. The primary objective of this 3-year project is to develop a basic scientific (thermodynamic) understanding of actinide volatilization and partitioning/speciation behavior in the thermal processes that are central to DOE/EM's mixed waste treatment program. The work is a combination of experimental studies and thermodynamic modeling. Transpiration and mass spectrometric measurements will be made to determine U, Pu and possibly Am volatile species and the extent of their volatilization when UO_2/U_3O_8, PuO_2 and AmO_2 are heated to temperatures of 500 to 1600°C under (i) pyrolyzing (reducing) conditions, and (ii) oxidizing conditions (i.e. $O_2(g) + H_2O(g)$ mixtures) in the presence of chlorine ($Cl_2(g)$ or $HCl(g)$). Work on uranium volatilization under reducing conditions will be performed in a laboratory at U.C. Berkeley in a collaboration with Professor D.R. Olander. In parallel with the experimental effort, a complete thermodynamic database for expected actinide gaseous species will be developed from literature data, from the proposed measurements, and from data predictions using bond energy correlation and statistical thermodynamics estimation methods.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Nuclear Materials problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Nuclear Materials".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
+ RL-TW04	C-169	Retrieval Project
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
+ RL-TW08	C-185	Process Waste Privatization Infrastructure
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
RF014	C-213	Industrial Zone Closure Project
+ SR-HL02	C-253	F-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
SR-HL05	C-265	Vitrification
+ SR-SW01	C-281	Consolidated Incinerator Facility
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in California

California Institute of Technology

55137-CA - Investigation of Novel Electrode Materials for Electrochemically-Based Remediation of High- and Low-Level Mixed Wastes in the DOE Complex

Year of Award: 1996 **Amount of Award:** $650,000
Problem Area: High Level Waste
Science Category/SubCategory: Inorganic Chemistry / Multiphase/Gaseous Chemistry
Principal Investigator: Dr. Nathan S. Lewis, 818-395-6335, nslewis@cco.caltech.edu
Major Collaborator(s): Marc A. Anderson at the University of Wisconsin
For More Information: http://www.doe.gov/em52/55137.html

Description Provided by Investigator:

One of the key issues that must be solved to achieve a successful remediation of the high level liquid wastes (HLW) at the Hanford and at Savannah River sites is the removal of the significant quantities of nitrate and nitrite in the existing liquid waste streams that are presently on these sites in the DOE complex. In addition, either prior to or after separation of the high level waste components (for eventual vitrification of the high level components), the Hanford waste stream has a substantial concentration of organics that must be processed in such a fashion that the organics are either removed entirely or are degraded into CO_2 or other benign carbon-containing materials. These process steps are needed so that the low level waste stream obtained after separation of the high level waste components (Cs and Sr, primarily) is suitable for conversion into grout (or possibly vitrified), which is now not feasible due to the high concentration of organic materials currently present in the existing liquid wastes.

One very promising method of waste stream remediation, which is the focus of this proposal, is electrochemical oxidation. Electrochemical oxidation is well-documented to have some significant advantages relative to high and low temperature steam oxidation processes, including the fact that electrochemical treatment is an in-situ remediation process whereas the water oxidation processes and most other proposed methods are pump-and-treat technologies. In fact, electrochemical degradation of nitrate, nitrite, and organic components in the DOE HLW streams or simulants thereof graded out very highly in a recent DOE assessment of potential remediation methods, with its main drawback relative to high temperature water oxidation processes merely being a lack of prior experience with the operation of electrochemical processes on the scale of, and under the harsh conditions anticipated to be present in, the radioactive waste environment of the DOE sites.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
§ SR-HL05	C-265	Vitrification
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
RF014	C-213	Industrial Zone Closure Project
+ SR-SW01	C-281	Consolidated Incinerator Facility
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in California

California Institute of Technology

55284-CA - Aquifer Transport of Th, U, Ra, and Rn in Solution and on Colloids

Year of Award: 1996 **Amount of Award:** $499,945
Problem Area: Remedial Action
Science Category/SubCategory: Geochemistry / Colloidal Chemistry and Transport
Principal Investigator: Dr. G. J. Wasserburg, 818-395-6439, isotopes@gps.caltech.edu
Major Collaborator(s): Mahalingam Baskaran at Texas A&M University
For More Information: http://www.doe.gov/em52/55284.html

Description Provided by Investigator:

The purpose of this study is to investigate the behavior of naturally occurring U, Th, Ra, and Rn isotopes in groundwater and to utilize these elements as natural analogues for waste radionuclides in predicting migration behavior in potentially impacted aquifers. The study will obtain information on the natural radionuclides provided to groundwater throughout an aquifer system that will be used to constrain quantitatively the transport in groundwater and removal to host formations of radionuclides that potentially may reach the recharge zones of these aquifers. There have been numerous investigations that have examined various aspects of the behavior of these nuclides. However, there have been two developments which open new avenues of investigation and allow outstanding issues to be considered.

Firstly, previous studies were largely based on analyses by counting techniques, which can provide precise data for only short-lived nuclides. Discussions regarding long-lived nuclides were based upon more limited data, especially for Th. In typical groundwater environments, the low solubility of ThO_2 and the surface reactivity of Th species result in concentrations as low as 10^{11} atoms ^{232}Th per liter and 10^6 atoms ^{230}Th per liter that have limited the studies of Th in groundwaters based upon counting methods. Utilizing techniques developed in our laboratory for the measurement of long-lived Th and U isotopes by mass spectrometry (Chen et al., 1986, Edwards et al., 1987), it is now possible to measure these low concentrations of Th in groundwaters (Banner et al., 1990, 1991). This also opens the possibility of conducting laboratory experiments of Th and U behavior that have only been conducted on short-lived nuclides. As discussed below, this includes measuring the rates of input to groundwaters by recoil, leaching, and dissolution.

Secondly, various recent investigations have focussed on the role of colloids in the migration of radionuclides. Ultrafiltration techniques have been developed that can be used for the separation of colloids, and the conditions under which radionuclides are significantly associated with organic and inorganic colloids can be examined. While the data regarding the association of long-lived nuclides with colloids is limited, we have found that ultrafiltration techniques can be used to process large volumes of water, allowing measurement of short-lived and long-lived nuclides in ultrafiltered waters and colloid separates (Porcelli et al., 1996).

The goal of the proposed work is to investigate the fundamental controls on natural radionuclide migration in specific aquifers by integrating aquifer sample analyses, focussed laboratory experiments, and field observations of two aquifer study sites. This will include analyses of particles and colloids as well as 'dissolved' species. The work will use standard decay counting methods for determining concentrations of the short-lived nuclides and high precision mass spectrometry to measure the long-lived nuclides.

The project will focus on obtaining the following:

1. Measurements of radionuclide concentrations in groundwaters and changes in concentrations along groundwater flow lines as water chemistry evolves.
2. Measurements of the proportion of radionuclides transported by colloids and particles.
3. Laboratory measurements of the rate of recoil supply of radionuclides to groundwater.
4. Measurement of the distribution of parent elements within the aquifer rock to determine the controls on radionuclide recoil and dissolution inputs to groundwater.

5. Calculation of radionuclide removal and retardation rates based upon input rates and groundwater evolutionary history.
6. Laboratory measurements of the rates of removal by adsorption of the radionuclides onto aquifer host rocks, and comparison of this data with calculated aquifer removal rates.
7. Model calculations and predictions of the transport behavior and rates of migration of waste radionuclides that potentially may reach the recharge zones of sandy and limestone aquifers.

There are a range of U, Th, Ra, and Rn isotopes in the ^{238}U and ^{232}Th decay series that will be included in the proposed work. These are (with half-lives),

In the ^{238}U decay series:
^{238}U (4.49 x 10^9y), ^{234}Th(24.1d), ^{234}U (2.48 x 10^5y),^{230}Th(7.52 x 10^4y), ^{226}Ra(1602y), ^{222}Rn(3.83d) and in the ^{232}Th decay series:
^{232}Th (1.39 x 10^{10}y), ^{228}Ra(5.75y),^{228}Th(1.913y),^{224}Ra(3.64d), ^{220}Rn(56sec)

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ AL007	C-7	Environmental Restoration
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV212	C-49	Underground Test Area (UGTA)
§ NV214	C-53	Industrial Sites
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in California

Stanford University

54666-CA - Mechanisms, Chemistry, and Kinectics of Anaerobic Biodegradation of Cis-Dichloroethylene and Vinyl Chloride

Year of Award: 1996 **Amount of Award:** $686,205
Problem Area: Remedial Action
Science Category/SubCategory: Microbial Science / Biodegradation and Biotransformation
Principal Investigator: Dr. Perry L. McCarty, 415-723-4131, mccarty@cive.Stanford.EDU
For More Information: http://www.doe.gov/em52/54666.html

Description Provided by Investigator:

Background and Significance

This three year research project will study the anaerobic biological conversion of cis-1,2-dichloroethene (cDCE) and vinyl chloride (VC) to ethene. The study will be conducted in three separate phases, the first to better understand the mechanisms involved in cDCE and VC biodegradation, the second to evaluate the chemistry of the processes involved, and the third, to study factors affecting reaction kinetics. The following contains a brief background to establish the programmatic need for the study, research objectives, methods of accomplishment, and a summary of the principal investigator's publication and research backgrounds. The DuPont Chemical Company is highly interested in this study because of its importance to their program for in-situ anaerobic bioremediation of chlorinated solvent contaminants in groundwater, and has agreed to directly cost-share on the research at a rate of $75,000 per year for the three year period.

Programmatic Need for Study

The chlorinated solvents, trichloroethene (TCE), tetrachloroethene (PCE), and carbon tetrachloride (CT) have been widely used by industry, the Department of Defense, and the Department of Energy as solvents for cleaning. Through leakage and poor disposal practices, these solvents have become the most frequent groundwater contaminants throughout the country, causing one of the most difficult and costly contamination problems for remediation. Significant groundwater contamination with these solvents exist at DOE facilities such as Savannah River, Hanford, and the Idaho National Engineering Laboratory. Most remediation approaches involve the extraction of contaminated groundwater and its cleanup at the surface through expensive physical and/or chemical methods. However, anaerobic biological processes have resulted in the natural destruction of the chlorinated solvents (intrinsic bioremediation) in some cases (EPA, 1994; Hinchee, et al., 1995b). Engineered in-situ biodegradative processes also offer much promise for complete destruction in others (Hinchee, et al., 1995a). The processes are highly complex and additional basic research on the biological processes involved is essential both for evaluating the true potential for intrinsic bioremediation at some sites and for reliable engineering of the process at others.

The biological anaerobic reduction of chlorinated aliphatic hydrocarbons (CAHs) such as PCE and TCE to cDCE and VC in groundwater was reported in the early 1980s. Further reduction of PCE and its intermediates to ethene was reported in 1989. Several pure cultures of anaerobic bacteria have been found to reductively dehalogenate PCE to cDCE. Rates of reduction of PCE and TCE to cDCE are high and the need for electron donor addition for the reactions is small.

However, the subsequent reduction of cDCE to VC, and then of VC to the harmless end product, ethene, is much slower and only recently has a pure culture been reported that is capable of reducing cDCE to VC or VC to ethene. There are numerous reports of such conversions in mixed cultures. This area is where basic research is most in need, and thus the subject of this research. We have highly active mixed cultures obtained from DuPont's Victoria, Texas, site that convert PCE completely to ethene and will use these cultures in the proposed studies.

Research Objectives

The objectives of this study are to (1) determine the biochemical pathways for reductive dehalogenation of cDCE and VC, including identification of the enzymes involved, (2) determine the chemical requirements, especially the type and quantity of electron donors needed by the microorganisms for reductive dehalogenation, and (3) evaluate the kinetics of the process with respect to effect of concentration of both the electron donors and the electron acceptors (cDCE and VC).

The evidence available from pure cultures indicate that reductive dehalogenation is coupled with energy production, an observation that suggests it may be an efficient mechanism for PCE and TCE dehalogenation. These studies also suggest that hydrogen may be a key intermediate in the anaerobic catabolism of organics that is used by the dehalogenating bacteria as an electron donor for dehalogenation. A general observation is that yeast extract is required to satisfy trace organic nutrient requirements, and an organic carbon source such as acetate is required for general cell synthesis. Such a hypothesis suggests that the dehalogenating microorganisms would occupy a niche in an anaerobic system somewhat similar to that occupied by the hydrogen-consuming methanogens, sulfidogens, and acetogens. Here, complex organics are fermented to simpler compounds, which are then oxidized further by removal of hydrogen and associated electrons. The hydrogen is an end product of such oxidation, and for methanogenesis, acetogenesis, and/or sulfidogenesis (sulfate reduction), is used as an electron donor. Evidence is accumulating that the dehalogenating bacteria also compete for such hydrogen, thus are part of a complex ecological system.

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Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§ RL-ER08	C-147	Groundwater Management
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in California

Stanford University

54860-CA - Sorption of Heavy Metals and Radionuclides on Mineral Surfaces in the Presence of Organic Co-Contaminants

Year of Award: 1996 **Amount of Award:** $784,220
Problem Area: Remedial Action
Science Category/SubCategory: Geochemistry / Sorption/Desorption
Principal Investigator: Dr. James O. Leckie, 415-723-2524, leckie@cive.Stanford.EDU
Major Collaborator(s): George Redden at Stanford University
For More Information: http://www.doe.gov/em52/54860.html

Description Provided by Investigator:

A review of the known inventory of chemical wastes at DOE facilities reveals that a large fraction of the waste is present as complex mixtures containing radionuclides, heavy metals, fuels, oils, organic solvents, and a variety of organic metal complexing agents (Riley and Zachara 1992). This situation is a result of a history of co-disposing wastes associated with chemical processing, metal surface cleaning, decontamination, and fabrication procedures used in the production of nuclear fuels and weapon components. Similar conditions also exist in industry where mixed wastes with heavy metals and chelating agents have been produced. The large inventory of complex and potentially unstable wastes must be stored until suitable treatment, confinement or disposal technologies have been developed. Unfortunately, in many cases the waste materials have been either discharged directly into open pits, or have since escaped from temporary containment facilities and now contaminate surrounding soils and groundwater.

The chemical complexity of these wastes present particularly challenging problems with respect to predicting subsurface migration of the radionuclides and heavy metals, and developing suitable remediation strategies. Among the organic compounds at DOE sites are a number of organic chelating agents that can form stable solution complexes with metals, radionuclides, and their oxy-ions. Examples include EDTA[1], NTA[2], and citric acid. It would be reasonable to predict that the formation of metal-organic complexes, especially those with stable multi-dentate structures, will influence the mobility of the metals and radionuclides in soils and groundwater. A general prediction that is consistent with the few available field studies would be that metal complexing organic ligands should increase metal mobility. This has already been demonstrated in a number of studies (e.g., Means et al., 1978; Girvin et al., 1993; Zachara et al., 1995). However, recent work with uranium and citric acid (Redden et al., 1996) and cadmium and citric acid (Boily and Fein, 1996) on metal oxides has shown that, under particular chemical conditions, complexing agents can actually enhance metal adsorption. Mobility of ionic solutes in groundwater is a function of the extent of partitioning between the mobile (water) and immobile (soil, mineral) phases. Organic ligands compete with reactive surface binding sites for metal solutes, or bind directly to surfaces thereby altering the type and availability of binding sites. In most field applications, increased mobility of soil and groundwater contaminants is not desirable since retrieval of the contaminants or isolating the public from hazardous conditions becomes more difficult as zones of contamination expand. However, in some cases, where remediation involves contaminant recovery, maximum mobility can be a distinct advantage.

At present, with the available experimental database, broad generalizations concerning the effect of organic ligand and chelating agents on metal or radionuclide mobility cannot be made. The quantitative predictions of partitioning that are necessary to estimate contaminant transport are not yet possible, and specific details of the chemical mechanisms are still hypothetical. In order to make reasonable transport predictions, an expanded database is needed for a range of priority heavy metal contaminants, common ligands, and representative mineral surfaces. Elucidating the mechanisms by which organic ligands affect metal partitioning at surfaces will provide information necessary for the design of effective treatment strategies.

[1] Ethylenediaminetetraacetic acid
[2] Nitrilotriacetic acid

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Project ID	Page #	Project Title
§ AL007	C-7	Environmental Restoration
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV212	C-49	Underground Test Area (UGTA)
§ NV214	C-53	Industrial Sites
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ OR-48101	C-99	Offsite Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
SR-HL03	C-257	Waste Removal Operations and Tank Closure

Environmental Management Science Program Research in California

University of California at Berkeley

54546-CA - Engineered Antibodies for Monitoring of Polynuclear Aromatic Hydrocarbons

Year of Award: 1996 **Amount of Award:** $890,930
Problem Area: Health / Ecology / Risk
Science Category/SubCategory: Health Science / Molecular, Structural and Genomic Science
Principal Investigator: Dr. Alexander E. Karu, 510-643-7746, hyblab@socrates.berkeley.edu
Major Collaborator(s): Victoria Roberts at Scripps Research Institute
Qingxiao Li at the University of Hawaii, Manoa
For More Information: http://www.doe.gov/em52/54546.html

Description Provided by Investigator:

Objectives

The objective of this multidisciplinary project is to use molecular biological techniques to derive a set of antibodies with useful affinities and selectivities for recovery and detection of polynuclear aromatic hydrocarbons (PAHs) in environmental and biological samples. The long-term goal is to develop immunodetection methods that will be useful in biomarker research and regulatory monitoring of PAHs.

Rationale for the approach

Immunoaffinity and immunoassay methods are increasingly being used worldwide to detect and estimate amounts of man-made pollutants and toxic natural products. The use of monoclonal antibodies (MAbs) improved the performance and reliability of many of these methods. The present generation of hazardous substance immunoassays uses antiserum or a single MAb to recognize individual analytes or a group of similar analytes. Future assay formats such as sensor arrays will employ panels of antibodies to identify multiple analytes using cross-reactivity pattern recognition. We are using recombinant antibody methods that offer new ways to obtain antibodies with useful cross-reactivity patterns for PAHs and similar compounds.

Polynuclear aromatic hydrocarbons (PAHs) are environmental contaminants of concern to DOE. The effects of PAHs on mammals, fish, birds, invertebrates, and microorganisms have been extensively studied, and several microbial systems have been developed for PAH bioremediation. Individual PAHs vary greatly in their abundance, toxic and carcinogenic potency and environmental impact. Some PAH metabolites form adducts on proteins and DNA that are potential biomarkers of exposure or defective repair. There are about 70 isomeric forms of the PAHs that have 4 to 6 fused rings. Commercial immunoassays are now available to detect the most abundant PAHs. It would be much more valuable to have immunoassays that could distinguish subclasses, such as the 3, 4, and 5-ring PAHs, or the major carcinogenic species. However, the analogs are so similar that it would be prohibitively difficult and costly to prepare numerous different immunizing and screening haptens and attempt to derive hybridoma antibodies with the desired selectivities.

Our research approach is to recover the genes of useful antibodies, express them in bacteria, develop 3-dimensional structural models to visualize antibody-antigen interactions, and then derive improved variants by directed and combinatorial mutagenesis. A recombinant antibody's affinity, selectivity, and other physical, chemical and structural properties may be changed to make it a more suitable analytical tool. We recently cloned and expressed recombinant Fab fragments that competitively bind 3, 4, and 5-ring PAHs. We will develop models of the combining sites to guide the design of mutants with altered functions. We will also search for PAH-specific recombinant Fabs or single-chain Fv antibodies (ScFvs) by screening the latest generation of immensely diverse combinatorial Fab and ScFv phage display libraries on selected PAH haptens. This should yield antibodies with sufficiently distinct binding properties for pattern recognition, without the need for conventional immunization, animal use, and hybridoma development.

An important part of this research is the work Dr. Li's laboratory will undertake to integrate recombinant antibodies with practical, reliable sample preparation and cleanup methods. We will attempt to find antibody engineering solutions for problems that Dr. Li may encounter using the antibodies for real-world analytical chemistry.

We are now in a unique position to investigate which amino acids and secondary structures in the antibody's combining site govern PAH recognition. During the past year, we derived two recombinant Fab antibodies that competitively bind benzo(a)pyrene, pyrene, phenanthrene, chrysene, and other PAHs in solution. The cross-reactivity profiles of these Fabs with PAHs are subtly different, but their sequences differ in 23 amino acids. About half of these are in complementarity-determining region (CDR) loops L1, L2, H2, and H3. By analysis of the sequence differences of these two Fabs in the context of their 3-dimensional structures, we will ascertain which amino acid side chains are crucial for antigen recognition. These side chains will be altered by *in vitro* mutagenesis to predictably modify the binding pockets so that they specifically recognize classes of PAHs.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Health / Ecology / Risk problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Health / Ecology / Risk".

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Project ID	Page #	Project Title
AL007	C-7	Environmental Restoration
+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
NV212	C-49	Underground Test Area (UGTA)
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
RL-ER08	C-147	Groundwater Management
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in California

University of California at Berkeley

54655-CA - Collaborative Research: Hydrogeological-Geophysical Methods for Subsurface Site Characterization

Year of Award: 1996 **Amount of Award:** $920,822
Problem Area: Remedial Action
Science Category/SubCategory: Geophysics / Subsurface Imaging
Principal Investigator: Dr. Yoram N. Rubin, 510-642-2282, rubin@arimor.ce.berkeley.edu
Major Collaborator(s): Dr. Gary Mavko at Stanford University
For More Information: http://www.doe.gov/em52/54655.html

Description Provided by Investigator:

This project focuses on three issues that are critical to Environmental Management of contaminated sites: reducing cost, reducing risk, and increasing the effectiveness of subsurface remediation schemes. The significance of this research is that it addresses the issue of site characterization: not only that this issue is a very significant budget item in the site clean-up effort, but also that it is now realized that accurate and reliable site characterization is the key to the success of any clean-up effort.

Our objective is to develop the scientific basis and demonstrate methodologies for inexpensive high resolution imaging of natural heterogeneities and for relating these heterogeneities to the hydrogeologic parameters that control flow and contaminant transport - in effect, to develop methods for "imaging" hydrogeologic parameters. Our focus is to help establish the scientific basis for applying shallow geophysics to hydrogeological problems, through (a) feasibility studies, (b) sediment-rock physics, (c) improvements in the procedures for co-interpretation of geophysical and hydrogeological data, and ultimately, (d) demonstration of a practical implementation of joint seismic and electromagnetic data for hydrogeologic characterization of DOE contaminated sites. An essential task will be to identify limitations, pitfalls, and uncertainties of these co-interpretations -i.e., to quantify the risks in applying shallow geophysics to hydrogeological site characterization. The research combines theoretical modeling, field data processing, analysis of laboratory measurements, and integration techniques.

Our approach is to use seismic and electromagnetic methods jointly to map the distribution of seismic velocity and attenuation and electrical conductivity in the 3-D volume defined by a set of boreholes. In a rough sense both velocity and conductivity depend on porosity and to a lesser extent on permeability, clay content, saturation and nature of pore fluid. Laboratory studies have shown these relationships in great detail and we now are refining these results and utilizing them to interpret survey data in terms of maps of the distribution of the hydrogeologic properties.

This is an interdisciplinary study, since it integrates the fields of hydrogeology and geostatistics, geophysics, and rock physics. The team of researchers brings to this project a large collective experience in performing theoretical, field and lab work.

This work is an extension of research being carried out in the Subsurface Science Program with the DOE Office of Health and Environmental Research, and it complements the research on High Resolution Geophysical Imaging for Subsurface Process Definition by E.L. Majer from LBL.

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Project ID	Page #	Project Title
+ RL-TW05	C-173	Process Waste Support
+ RL-TW07	C-181	Process Waste Privatization Phase II
+ SR-HL01	C-249	H-Tank Farm
+ SR-HL02	C-253	F-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in California

University of California at Berkeley

54656-CA - Mixing Processes in High-Level Waste Tanks

Year of Award: 1996 **Amount of Award:** $416,830
Problem Area: High Level Waste
Science Category/SubCategory: Engineering Science / Design, Process and Modeling
Principal Investigator: Dr. Per F. Peterson, 510-643-7749, peterson@nuc.berkeley.edu
For More Information: http://www.doe.gov/em52/54656.html

Description Provided by Investigator:

Flammable gases can be generated in DOE high-level waste tanks, including radiolytic hydrogen, and during cesium precipitation from salt solutions, benzene. Under normal operating conditions the potential for deflagration or detonation from these gases is precluded by purging and ventilation systems, which remove the flammable gases and maintain a well-mixed condition in the tanks. Upon failure of the ventilation system, due to seismic or other events, however, it has proven more difficult to make strong arguments for well-mixed conditions, due to the potential for density-induced stratification which can potentially sequester fuel or oxidizer at concentrations significantly higher than average. This has complicated the task of defining the safety basis for tank operation, and in the case of cesium precipitation, has led to delays in cesium processing which are quite expensive. Improved tools for predicting tank mixing processes following loss of ventilation, coupled with mixing experiments designed specifically for DOE waste tank conditions, have the potential to both strengthen the safety basis for tank operation and to prevent schedule delays in tank operations.

Currently no numerical tools exist for modeling the transient evolution of fuel and oxygen concentrations in waste tanks following loss of ventilation. When used with reasonable grid resolutions, standard multi-dimensional fluid dynamics codes suffer from excessive numerical diffusion effects, which strongly over predict mixing and provide nonconservative estimates, particularly after stratification occurs. The National Institute of Standards and Technology (NIST) has developed useful codes for predicting stratification and mixing due to fires in enclosures, but these codes are not supported by appropriate experiments for waste tanks and do not consider mixing induced by injected jets or the detailed distribution of fuel and oxygen concentration.

We propose a concentrated effort to develop models and a numerical tool BMIX (Berkeley Mechanistic Mixing Model) to mechanistically predict mixing processes in large waste-tank volumes, where mixing processes can be driven by hot and cold vertical and horizontal surfaces and injected buoyant jets. We will support the model with scaled experiments using simulant fuels (helium and refrigerant-22 for hydrogen and benzene) to study the specific mixing processes which occur in waste tanks, and will also support the implementation of the code for use in waste tank operation.

Over the previous two years, we have developed the necessary scaling and analytical models to predict the transition from well-mixed to thermally stratified conditions in large enclosures, and have validated these models against both experimental data and high-resolution, multidimensional computational fluid dynamics (CFD) predictions. It appears that we can now describe, with good accuracy, mixing and transport processes in large complex enclosures, using simple coupled one-dimensional differential equations. Supported by specific experiments, these coupled equations can be solved with minimal computational expense.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

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Project ID	Page #	Project Title
§+ RL-TW04	C-169	Retrieval Project
§+ RL-TW05	C-173	Process Waste Support
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations

Environmental Management Science Program Research in California

University of California at Davis

54681-CA - Dynamics of Coupled Contaminant and Microbial Transport in Heterogeneous Porous Media

Year of Award: 1996 **Amount of Award:** $2,035,829
Problem Area: Remedial Action
Science Category/SubCategory: Microbial Science / Microbial Transport
Principal Investigator: Dr. Timothy R. Ginn, 509-372-6075, trginn@ucdavis.edu
Major Collaborator(s): Dr. Ellyn M. Murphy at Pacific Northwest National Laboratory
Dr. John H. Cushman at Purdue University
Dr. Madilyn Fletcher at the University of South Carolina
For More Information: http://www.doe.gov/em52/54681.html

Description Provided by Investigator:

Dynamic microbial attachment/detachment occurs in subsurface systems in response to changing environmental conditions caused by contaminant movement and degradation. Understanding the environmental conditions and mechanisms by which anaerobic bacteria partition between aqueous and solid phases is a critical requirement for designing and evaluating in situ bioremediation efforts. This interdisciplinary research project will provide fundamental information on the attachment/detachment dynamics of anaerobic bacteria in heterogeneous porous media under growth and growth-limiting conditions. Experiments will provide information on passive and active attachment/detachment mechanisms used by growing anaerobes capable of reductive dechlorination. Theoretical representations of these attachment/detachment mechanisms will be incorporated into existing flow and transport models that incorporate heterogeneity effects and can be used to predict behavior at field scales. These mechanistic-based models will be tested against experimental data provided through controlled laboratory experiments in heterogeneous porous media in large (meter) 2-D flow cells.

The multidisciplinary team contributing to this project has evolved from previous collaborations under DOE's Subsurface Science Program and provides strong expertise in bacterial adhesion mechanisms and transport, physiology and phylogeny of methanogenic bacteria, bioreactive transport theory in heterogeneous porous media, and process scaling. In addition to a mechanistic-based predictive model, this research will lead to new theories for the transient spatial distribution of microbial populations and contaminant plumes in heterogeneous porous media, improving our capability for designing staged remediation strategies for dealing with mixed contaminants.

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§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§ RL-ER08	C-147	Groundwater Management
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in California

University of California at Davis

54890-CA - On-Line Slurry Viscosity and Concentration Measurement as a Real-Time Waste Stream Characterization Tool

Year of Award: 1996 **Amount of Award:** $691,154
Problem Area: High Level Waste
Science Category/SubCategory: Engineering Science / Diagnostics
Principal Investigator: Dr. Robert L. Powell, 916-752-8779, rlpowell@ucdavis.edu
Major Collaborator(s): Reza Shekarriz at Pacific Northwest National Laboratory
For More Information: http://www.doe.gov/em52/54890.html

Description Provided by Investigator:

The radioactive and mixed wastes currently stored in the 177 underground storage tanks at the Hanford Site of the U. S. Department of Energy are complex mixtures of insoluble sludge, soluble salts, and supernatant liquids. In most of the double-shell tanks, the insoluble sludge layer, comprised of densely packed and networked solid particles, exceeds one third of the total volume of waste. The slurries pumped from the tanks will require pretreatment steps to separate the waste into different categories (high level, low level, etc.) for appropriate disposal and treatment. It is planned to transport the waste to various processing plants, separation facilities, and among different storage tanks using cross-site transfer pipelines. The long-term remediation strategy calls for disposal of the high-level waste in deep geologic repositories in the form of vitrified glass.

The current perception is that high safety factors during transport can be maintained by diluting the waste slurries to obtain low viscosity mixtures. These can easily be transferred across the pipelines to the processing plants or other tanks. However, this option is not favored due to the high cost associated with separation of a higher volume of liquid from the mixture in the separation plants. Clearly, this is not a waste minimization strategy. Additional processing will be required for the diluent which itself can become a waste. In this case, waste minimization is directly related to the ability to transport the waste with little or no dilution under tightly controlled conditions. The need for careful evaluation of the waste transfer process via pipelines is recognized. Five of the six existing cross-site transfer lines between the 200 West and 200 East areas of Hanford Site have been plugged by the slurries). Replacement transfer pipelines are currently being constructed. New methodologies are being developed to reduce risk associated with equipment loss and plugging of the pipelines during transfer. One of the most important steps in defining these criteria is *property measurement and characterization* of the waste. The current plan is for off-line measurement of the properties of the waste. This process is expected to be time-consuming and extremely expensive over the lifetime of the project.

Elemental analysis of tank sludges reveal that the major insoluble components expected to be present are oxides and hydroxides of Al, Fe, Zr, and Cr, insoluble salts such as calcium phosphates, and aluminosilicate minerals. Transmission electron micrographs of some tank sediments show that nanoparticles of many phases are present, and they reveal that over 50% of the insoluble material in some of the tank sludges are smaller than 1 æm and composed of colloidal particles. It has been shown that these particles form aggregates or clusters and that the size of the clusters depends on the particle composition, solution pH, ionic strength, concentration of solids, shear rate, and temperature. Further, it has been shown that suspension properties strongly depend on primary particle size, cluster size, and fractal dimension of the clusters. Given the strong dependence of the rheological properties on the environment under which the clusters exist, off-line measurements of the rheological properties have been under critical scrutiny. For example, once a sample is withdrawn from the process stream, its rheological (flow) properties will begin to change. Further, given that the material in the pipeline may not be homogeneous, it will be difficult to obtain a representative sample.

The proposed work seeks to directly address the need for a robust technique to provide a comprehensive characterization of the relevant rheological properties under actual processing conditions to permit the monitoring and control of transport tank slurries. The principal thrust is to address the issue of on-line viscosity measurement by examining two potential viable technologies, nuclear magnetic resonance imaging (NMRI) and acoustic velocimetry. We focus on the fundamental scientific issues that must be overcome in order to implement these techniques. This effort consists of a collaboration between the University of California at Davis (UCD) and Battelle Pacific Northwest National Laboratory (PNNL). Each organization brings specific expertise to the project. UCD has a strong background in the application of NMRI to fluid mechanics while PNNL has the needed expertise in acoustic velocimetry. Further the collaboration assures that the focus on the tank retrieval and waste problems at the Hanford site will be maintained, as will the active consultation of engineers at the principal contractor at Hanford, presently, Westinghouse. In this regard, Dr. Harry Babad of Westinghouse Hanford Company has agreed to act as an advisor to the project. Dr. Babad is the science advisor to Dr. Susan J. Eberlein (manager of the Tank Waste Remediation Systems Technical Basis Group) and he is currently involved in the planning and guidance for the retrieval process, sluicing and waste transfer, of tank wastes.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§+ RL-TW04	C-169	Retrieval Project
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
§ SR-HL05	C-265	Vitrification
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
RF014	C-213	Industrial Zone Closure Project
+ SR-SW01	C-281	Consolidated Incinerator Facility

Environmental Management Science Program Research in California

University of California at Davis

55118-CA - Plant Rhizosphere Effects on Metal Mobilization and Transport

Year of Award: 1996 **Amount of Award:** $454,904
Problem Area: Remedial Action
Science Category/SubCategory: Plant Science / Plant Metabolism
Principal Investigator: Dr. Teresa W.-M. Fan, 916-752-1450, twfan@ucdavis.edu
Major Collaborator(s): David Crowley at the University of California at Riverside
For More Information: http://www.doe.gov/em52/55118.html

Description Provided by Investigator:

Among the factors that influence metal availability to soil-grown plants, one of the least understood is the influence of root/soil interfaces on metal mobilization and subsequent transport into the root. These include root exudation for chelating and reducing metal ions, cell wall binding of metal ions, and root-microbial associations. Past research efforts, aimed largely at understanding plant iron deficiency, have focused on specific chelating agents that are released by plant roots and microorganisms to facilitate iron solubilization and uptake (Crowley and Gries, 1994; Manthey et al., 1994). Although there have been some hints that root exudation may also govern mobilization and transport of other trace metals, a mechanistic understanding of the process for mobilization of metals other than iron is lacking. Any progress in this area will first require identifying root exudate and cell wall components which may serve as metal chelating or reducing agents. It is also necessary to examine microbial metabolites, such as siderophores that are released into the rhizosphere, and the alteration of root exudates by root associated microorganisms. In this research, we propose a comprehensive profiling of root exudate and cell wall components that will greatly facilitate the identification of metal mobilizing compounds, and will study the composition of metal mobilizing substances in the rhizosphere as affected by mycorrhizae and other soil microorganisms.

The first objective of the research will be to determine the biochemical composition of root exudates, with a particular focus on metal-binding organic acids, and changes in their composition and biosynthesis in response to selected metals. Since grasses are considered to have many desirable characteristics for use in bioremediation, and produce phytosiderophores that are known to mobilize various metals, we will use wheat (*Triticum aesstivum)* as a model plant species. For our initial experiments, we will characterize the effects of selected metals on root exudates released by plants in hydroponic culture. The second objective will be to apply the analytical methodology developed in Objective 1 to investigating the influence of mycorrhizae on root exudation and metal uptake from heavy metal contaminated soil (e.g. soils from McClellan Air Force Base, Sacramento, CA) in soil microcosms. These objectives will be met through the accomplishment of three tasks:

(1) application of GC-MS and NMR techniques for comprehensive analysis of root exudate composition and biosynthesis over a range of metal concentrations for four micronutrients (Cu, Mn, Zn, and Ni) and two common metal pollutants (Cd and Al).

(2) cell wall structure and fragment analysis of roots as a function of exposure to different concentrations of the selected metals.

(3) soil microcosm experiments to investigate the effect(s) of soil microorganisms and mycorrhizae on (1) and (2).

Once root exudates or cell wall components that are involved in metal mobilization and/or transport are identified, it should be feasible to examine the metabolic control of their synthesis in future studies and to determine how microbial associations can affect this aspect of plant metabolism. Results from such research efforts should provide fundamental understanding of how soil-grown plants can be adapted for better performance in sequestering metal contaminants. An immediate benefit will be the development of methodology for rapid screening of plant varieties which may have enhanced metabolic capacity for metal mobilization and tolerance, and for examining enhancement of metal mobilization and uptake via plant breeding, manipulation of plant growth conditions, or microbial inoculation. Knowledge gained from this research should have direct applications to the design of plant-based remediation or restoration efforts.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§ RL-ER08	C-147	Groundwater Management
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in California

University of California at Los Angeles

54914-CA - Atmospheric-Pressure Plasma Cleaning of Contaminated Surfaces

Year of Award: 1996 **Amount of Award:** $1,212,000
Problem Area: Decontamination and Decommissioning
Science Category/SubCategory: Materials Science / Surface Chemistry
Principal Investigator: Dr. Robert F. Hicks, 310-206-6865, hicks@ea.ucla.edu
Major Collaborator(s): Dr. Gary Selwyn at Los Alamos National Laboratory
For More Information: http://www.doe.gov/em52/54914.html

Description Provided by Investigator:

Decommissioning of transuranic waste (TRU) into low-level radioactive waste (LLW) represents the largest cleanup cost associated with the nuclear weapons complex. We are developing a low-cost technology for converting TRU into LLW based on the selective plasma etching of plutonium and other actinides from contaminated structures. Plasma etching has already been used to remove Pu films from materials. However, this process is operated under vacuum, making it both expensive and difficult to apply to many nuclear wastes. We have achieved a major breakthrough in this field by demonstrating the operation of a γ-mode, resonant-cavity, atmospheric-pressure plasma jet (APPJ). We have shown that this jet etches kapton at between 10 and 15 µm/hour, and tantalum at between 1 and 2 µm/hour. Etching occurs below 373 K, so that delicate materials will not be destroyed by this process. Our plasma jet may be used to selectively remove plutonium and other actinide elements by converting them into volatile compounds that are trapped by adsorption and filtration. Since the jet operates outside a chamber, many nuclear wastes may be treated, including machinery, duct-work, concrete and other building materials. We are carrying out a collaborative research program between the University of California, Los Angeles (UCLA), and Los Alamos National Laboratory (LANL) to characterize the novel chemistry and physics of the atmospheric-pressure plasma jet. At LANL, the source physics is be studied using Stark-broadening, microwave interferometry, and laser-induced fluorescence (LIF). The metastables, neutrals and radical species produced with mixtures of NF_3, CF_4, C_2F_6, O_2,He and Ar are being identified by LIF, optical emission spectroscopy (OES), laser Raman spectroscopy (LRS), coherent anti-Stokes Raman spectroscopy (CARS), and mass spectroscopy (MS). At UCLA, the elementary surface reactions of these species with tantalum and tungsten (surrogate metals for Pu) are being studied in ultrahigh vacuum using a supersonic molecular-beam coupled to the plasma jet. The surfaces are being characterized by x-ray photoemission (XPS), infrared spectroscopy (IR), low-energy electron diffraction (LEED), and scanning-tunneling microscopy (STM). In addition, plutonium etching experiments are being carried out at the Los Alamos Plutonium Facility, employing the process designs and operating procedures that we develop. Through this research, we are discovering the elementary chemical processes that control the rate and selectivity for etching Ta,W and Pu thin films with atmospheric-pressure plasmas. This work will enable the development of a new technology for the low-cost, environmentally-benign decommissioning of nuclear waste.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Decontamination and Decommissioning problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Decontamination and Decommissioning".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
§ OR-43204	C-77	ORNL Bethel Valley Deactivation and Decommissioning
§ OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
§+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
§+ RL-ER06	C-141	Decontamination and Decommissioning
§+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
§ RL-TP10	C-163	Accelerated Deactivation
RF014	C-213	Industrial Zone Closure Project

Environmental Management Science Program Research in California

University of California at Los Angeles

54926-CA - Novel Ceramic-Polymer Composite Membranes for the Separation of Hazardous Liquid Waste

Year of Award: 1996 **Amount of Award:** $360,000
Problem Area: Remedial Action
Science Category/SubCategory: Separations Chemistry / Ligand Design and Ion-exchange
Principal Investigator: Dr. Yoram Cohen, 310-825-8766, yoram@ucla.edu
For More Information: http://www.doe.gov/em52/54926.html

Description Provided by Investigator:

There is a growing need in the fields of remediation, hazardous chemical waste treatment, water treatment and pollution prevention for new processes capable of selectively separating and concentrating a target species, often present in dilute solution. Although membrane systems have been touted as the most probable means to achieve difficult liquid-phase separations, at a reduced energy consumption level relative to conventional technologies (e.g., distillation, extraction) selective membranes with adequate structural integrity and longevity are lacking. In order to meet the above challenge, the proposed project will focus on the development and demonstration of novel robust ceramic-supported polymer (CSP) membranes for organic-aqueous and organic-organic separations. The proposed CSP membranes will fabricated by modifying the pore surface of a ceramic support membrane via a graft polymerization process to form a thin layer of terminally anchored chains covalently bonded to the membrane pore surface. Through the selection of the polymerized polymer surface layer can be synthesized to impart specific separation properties to the membrane. Moreover, with the CSP membrane fouling can be significantly reduced by terminally anchored chains that minimize surface solute adsorption. The CSP membranes can also be fabricated as hybrid membranes for simultaneous ultrafiltration and metal ion removal (by surface anchored chelating agents or ion exchange sites).

It is expected that this project will lead to the demonstration of a new technology for the "tailor design" of a new class of selective and robust ceramic-supported polymer membranes. This new approach will allow the rapid deployment of task-specific membranes for remediation applications, recovery and recycle, effluent treatment, and selective replacement of energy intensive separation processes.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ NV214	C-53	Industrial Sites
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER02	C-129	200 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ RF014	C-213	Industrial Zone Closure Project
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
ID-HLW-101	C-29	High-Level Waste Pretreatment
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW04	C-169	Retrieval Project
+ RL-TW05	C-173	Process Waste Support
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
+ SR-HL01	C-249	H-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
SR-HL05	C-265	Vitrification
+ SR-SW01	C-281	Consolidated Incinerator Facility
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in California

University of California at Riverside

55061-CA - Fundamental Studies of the Removal of Contaminants from Ground and Waste Waters via Reduction by Zero-Valent Metals

Year of Award: 1996 **Amount of Award:** $380,000
Problem Area: Remedial Action
Science Category/SubCategory: Inorganic Chemistry / Solid/Solution Chemistry
Principal Investigator: Dr. J. A. Yarmoff, 909-787-5336, yarmoff@ucr.edu
Major Collaborator(s): Christopher Amrhein at the University of California at Riverside
For More Information: http://www.doe.gov/em52/55061.html

Description Provided by Investigator:

In an effort to remove trace contaminants from wastewaters and groundwaters, elemental iron is being used for the reductive dechlorination of solvents and the removal of toxic trace elements, such as Se, Cr, and U. Both *in situ* reactive barriers and above-ground reactors are being developed for this purpose. However, the design and operation of these treatment systems requires a detailed process-level understanding of iron/contaminant interactions. To date, studies of these reactions have focused on macroscopic measurements, and consequently very little is known about the basic surface chemical reactions of these toxic elements and solvents with the iron. In this research project, we address these issues via fundamental investigations of the interactions of the relevant chlorinated solvents, trace elements, and trace element-containing compounds with single- and poly-crystalline Fe surfaces. This work will provide a fundamental physical and chemical understanding of these interactions, which is critical for the development of cleanup techniques and procedures.

We will use UHV surface science techniques, which were initially developed for studies of heterogeneous catalysis and semiconductor processing, to determine the type of surface bonding and changes to the surface composition of the iron during contaminant removal. Surface studies enable:

- Preparation of atomically clean and smooth surfaces of a particular single crystal face
- A determination of the composition and structure of the starting surfaces
- A detailed compositional, structural, and chemical analysis of adsorbed surface reaction intermediates
- Identification and quantitative analysis of adsorbed and desorbed reaction products

These UHV studies will provide detailed and unambiguous mechanistic details concerning each individual reaction. We will begin with fundamental experiments on atomically clean, and well-oriented, single crystal Fe samples. Bonding of adsorbates to the Fe surface will be studied using both laboratory and synchrotron radiation-based photoelectron spectroscopies, as well as low energy electron diffraction (LEED), Auger electron spectroscopy (AES), thermal desorption spectroscopy (TDS) and impact collision ion scattering spectroscopy (ICISS).

Atomically clean Fe surfaces will be reacted in UHV with model compounds to delineate the reaction mechanisms that occur in the bulk processes. Reactants will include atomic species, such as Se, U and Cl, and gaseous compounds, such as SeF_6, H_2SeO_4 and CCl_4. In particular, we will investigate the pathway by which Fe catalyzes the reduction of these compounds. Next, co-reaction of these contaminant species with O_2 and H_2O will be investigated. Ultimately, we will develop a UHV-compatible wet reaction cell so that surface science techniques can be used to probe surfaces following reaction in aqueous solution. Included in this will be depth profiling to determine the effect of an iron oxide overlayer on the reaction.

In support of the surface studies, bulk chemical studies are being used to determine the factors that affect the rate of trace element reduction and precipitation from solution and the rate of solvent removal. Factors that are likely to be important include: pH, ionic strength (and chemical composition, such as Cl, SO_4, HCO_3, and Na concentrations), oxygen and carbon dioxide content, temperature, and dissolved organic carbon concentration. We will characterize the effects of iron pretreatment and aging on the rate of reaction. Several techniques will be used to identify the forms of the secondary products, such as iron oxyhydroxide precipitates and coprecipitated or adsorbed species. Samples of the reacted iron will be sequentially extracted to identify the amounts of precipitated Fe^{3+} that formed and associations of the contaminant with these phases. Scanning electron microscopy with ion microprobe will be used to identify morphological changes to the iron metal and to identify secondary products. Mineralogical changes will be measured using x-ray diffraction, N_2 BET surface area, and thermogravimetric analysis. Synchrotron based x-ray absorption spectroscopic techniques, such as near-edge x-ray absorption fine structure (NEXAFS) and extended x-ray absorption fine structure (EXAFS). NEXFAS can provide the oxidation state of the trace element in the iron samples while EXAFS provides the nearest neighbor coordination. Reactions with organics (such as carbon tetrachloride) will be monitored with a purge and trap gas chromatograph- mass spectrometer.

This work is a collaboration between Profs. J. A. Yarmoff (Physics) and C. Amrhein (Soil and Environmental Sciences) of the University of California, Riverside (UCR). We are combining the expertise of a surface scientist, who has much experience in the delineation of surface chemical mechanisms via an array of techniques, with an environmental scientist, who is intimately acquainted with the chemical problems associated with environmental cleanup. This unique collaboration will not only produce important results with respect to chlorinated solvent and trace element removal via zero-valent metals, but it will also provide a basis from which other investigations of the basic surface chemistry relevant to environmental cleanup can be addressed.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ OR-46301	C-107	Portsmouth Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in California

University of California at San Diego

55041-CA - Molecular Characterization of a Novel Heavy Metal Uptake Transporter from Higher Plants & its Potential for Use in Phytoremediation

Year of Award: 1996 **Amount of Award:** $483,121
Problem Area: Remedial Action
Science Category/SubCategory: Plant Science / Plant Membrane Transport
Principal Investigator: Dr. Julian I. Schroeder, 619-534-7759, julian@biomail.ucsd.edu
For More Information: http://www.doe.gov/em52/55041.html

Description Provided by Investigator:

Soils with high levels of heavy metals such as Cd, Cr and Pb are detrimental to human and animal health. Many human disorders have been attributed to environmental contamination by heavy metals. Removal of heavy metals from highly contaminated soils is therefore a very costly but necessary process that is currently being pursued. Excavation and re-burial of top layer soils is the current, relatively inefficient, approach for decontamination of specific sites. Recent research indicates that uptake of heavy metals into plants via the root system may provide a cost effective approach for decontamination of heavy metal-laden soils. Several mechanisms have been identified which allow detoxification of heavy metals once they have reached the inside of plant cells, including binding to chelating substrates and transporting heavy metals into the plant cell vacuoles which function as storage organelles. However, the molecular biological mechanisms by which heavy metals are transported across the plasma membrane into root cells remain completely unknown. It has been suggested that passive uptake by ion channels, by heavy metal transporters, and by conjugated-metal transporters together could allow concentration of heavy metals by approximately 10^5-fold inside plant cells with respect to soil concentrations. However, no information has been obtained regarding the plant cDNAs that encode plasma membrane transporters which are able to catalyze the uptake of heavy metals.

By pursuing a genetic approach, we have cloned a cDNA from wheat roots, named *PMT1*, that shows a novel primary structure and contains several hydrophobic putative membrane-spanning domains. Expression of the *PMT1* cDNA enhances the sensitivity of growth to Cd^{2+}. Furthermore, PMT-expressing yeast cells show enhanced uptake of Cd, Pb and Ca^{2+}. Isolation of the wheat root *PMT1* cDNA will allow us to address questions regarding mechanisms of heavy metal uptake across the plasma membrane of plant cells and may contribute to testing future bioengineering of heavy metal removal by plants. We propose studies which will test the following hypotheses:

1. PMT1 functions as a plasma membrane heavy metal and Ca^{2+} uptake transporter isolated from higher plant roots.
2. Overexpression of the PMT1 cDNA in plants can be used to enhance plasma membrane heavy metal uptake into plant tissues.

To test these hypotheses we suggest experiments with the following specific aims:

i. Characterize the selectivity of PMT1 for uptake of toxic heavy metals such as Cd, Pb, Cr, Cu and nutrients such as Ca^{2+} and Mg^{2+}. Competition among nutrient metals and heavy metals for uptake will further be studied.
ii. Determine whether PMT1 itself represents a metal transporting membrane protein. The plasma membrane localization of the PMT1 protein will be analyzed and structural mutations in PMT1 which enhance heavy metal uptake will be isolated using a genetic selection system in yeast.
iii. Low-stringency hybridizations will be used to determine whether PMT1 is a member of a larger gene family and RNA expression levels of PMT1s will be analyzed. PMT1 hybridization to mRNAs isolated from known heavy metal hyper accumulating plants will be pursued.
iv. PMT1 and PMT1 mutants that enhance heavy metal uptake will be overexpressed in transgenic plants to determine whether PMT1 expression can enhance heavy metal uptake. Transgenic PMT1 overexpressing plants will be quantitatively analyzed for growth phenotypes, and heavy metal and nutrient accumulation.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§ RL-ER08	C-147	Groundwater Management
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in California

University of California at San Francisco

59828-CA - Bioavailability of Organic Solvents in Soils: Input into Biologically Based Dose-Response Models for Human Risk Assessments

Year of Award: 1997 **Amount of Award:** $1,100,000
Problem Area: Health / Ecology / Risk
Science Category/SubCategory: Health Science / Risk Assessment
Principal Investigator: Dr. Ronald C. Wester, 415-476-2468, rcwester@ucsf.edu
For More Information: http://www.doe.gov/em52/59828.html

Description Provided by Investigator:

Remediation clean-up costs for soil contaminants on DOE sites vary dramatically with the level to which soil must be decontaminated. Although more is known about the uptake of neat chemicals, particularly solvents, through the skin, comparatively little is understood about the dermal bioavailability of solvents in soil, dust, sludge, sediment, etc. Fundamental research on the kinetics and bioavailability of solvent-laden soils will have an immediate impact on human health risk assessment by replacing conservative, default assumptions that assume contaminants in soil are well absorbed through human skin, reduce uncertainties in exposure/dose model paradigms, and in turn, serve to positively influence regulatory cleanup action levels. Depending on the contaminant and soil type, one or more orders of magnitude may be gained in acceptable risk levels at DOE sites.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Health / Ecology / Risk problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Health / Ecology / Risk".

Environmental Management Science Program Research in Colorado

National Institute of Standards &Technology - Boulder

60155-CO - Measurements and Models for Hazardous Chemical and Mixed Wastes

Year of Award: 1997 **Amount of Award:** $500,000
Problem Area: Mixed Waste
Science Category/SubCategory: Engineering Science / Design, Process and Modeling
Principal Investigator: Dr. Cynthia Holcomb, 303-497-3437, holcomb@boulder.nist.gov
For More Information: http://www.doe.gov/em52/60155.html

Description Provided by Investigator:

Mixed hazardous and low-level radioactive wastes are in storage at DOE sites around the United States, awaiting treatment and disposal. These hazardous chemical wastes contain many components in multiple phases, presenting very difficult handling and treatment problems. These wastes may be reactive, radioactive, corrosive, or flammable. Current facilities do not have the capacity or technology to handle most of this diverse waste inventory (approximately 167,000 cubic meters), let alone the additional wastes generated from continuing clean-up efforts. **The safe handling, accurate characterization, and cost-effective design of new treatment techniques require an accurate and comprehensive knowledge of basic thermophysical property information, including the chemical composition and density of the phases present.** Traditionally, the models available for complex systems like these have been limited to liquid phase chemistry, ignoring the equilibrium vapor present, densities, and the surface tension. The lack of comprehensive and accurate predictive models for the properties of hazardous chemical and mixed wastes represents a severe deficiency in the fundamental knowledge necessary to enable remediation efforts. We propose to develop models for the mixtures with more comprehensive property predictions that will enable the calculation of parameters crucial to separation process design (phase equilibria, pressure drops, and heat transfer properties).

The models developed will include a vapor phase equation of state for mixed solvents, a liquid phase mixed solvent electrolyte model, vapor and liquid density correlations, and surface tension correlations. The models will accurately represent the liquid phase chemistry, the vapor in equilibrium with the liquid, the identification of multiple liquid phases, the densities of the coexisting phases, the solid solubility, and the surface tensions of multi-component mixtures. Parameters for the models will be determined from measured data. The models will be optimized and thoroughly tested with the experimental measurements from this study. A representative waste mixture has been selected to provide the optimum information for the development of accurate models that have the capability to provide reliable predictions for complex mixtures based on the minimum amount of experimental measurements. The liquid phase model will be based on functional groups rather than chemical compounds to allow a straightforward extension of the model to systems with related components.

Most hazardous chemical and mixed wastes contain water, organic solvents, salts, and trace amounts of hazardous or radioactive components such as heavy metals or radionuclides. It is not possible to thoroughly measure the properties of all of the combinations that will be encountered in actual wastes due to the complexity of the systems. We have chosen to measure the properties and to model a representative system of water, acetone, isopropyl alcohol, and sodium nitrate. Acetone and isopropyl alcohol were selected to provide data for two solvents with distinctly different functional groups that are commonly used industrial solvents likely to be present in aqueous waste. Nitrate anions and sodium cations are the most common ions present in the hazardous chemical and mixed waste inventory. Thus, sodium nitrate was the salt chosen for the representative mixture.

Measurements will be performed to obtain vapor-liquid equilibria, surface tension, coexisting densities, and compressed liquid densities for the representative mixture. The data will cover the temperature range of 275 to 425 K and pressures to 14 MPa. Vapor-phase density and vapor composition data for these types of systems are presently scarce or non-existent in the literature. Our unique capability of measuring a wide variety of thermodynamic properties in state-of-the-art apparatus will allow us to provide currently unavailable data that will serve as the foundation for the new models. Once developed, the thermodynamic models will form the basis for designing mixed waste separation and destruction processes (for example stripping columns, membrane separations, and liquid-liquid extractors) for which no design data have previously been available.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW03	C-287	Mixed Low Level Waste Project
+ RL-TW06	C-177	Process Waste Privatization Phase I
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Colorado

United States Geological Survey

60162-CO - Enhancements to and Characterization of the Very Early Time Electromagnetic (VETEM) Prototype Instrument and Applications to Shallow Subsurface Imaging at Sites in the DOE Complex

Year of Award: 1997 **Amount of Award:** $820,000
Problem Area: Remedial Action
Science Category/SubCategory: Geophysics / Subsurface Imaging
Principal Investigator: Dr. David L. Wright, 303-236-1381, dwright@musette.cr.usgs.gov
Major Collaborator(s): Dr. Weng C. Chew at the University of Illinois at Urbana-Champaign
For More Information: http://www.doe.gov/em52/60162.html

Description Provided by Investigator:

The U.S. Geological Survey and the University of Illinois propose to improve the state-of-the-art of electromagnetic imaging of the shallow (0 to 5 m) subsurface in conductive media with potential applications to subsurface characterization, landfill stabilization, decontamination/decommissioning, and waste characterization at sites in the DOE complex. We plan to accomplish the research objectives by a combination of hardware and software enhancements to the existing Very Early Time Electromagnetic (VETEM) prototype instrument, physical modeling experiments, numerical forward and inverse modeling, and field demonstrations. We will enhance the existing system with additional antennas, additional transmitter options, probably one or more gradiometer configurations, and a modified receiver. The instrument enhancements will be guided by numerical forward, inverse, and antenna modeling. We propose to develop fast forward and inverse modeling codes appropriate to the VETEM instrument in 1D and, if possible, 2D that will run on a PC for in-the-field interpretation, as well as more detailed post-processing models.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ NV214	C-53	Industrial Sites
§ RF014	C-213	Industrial Zone Closure Project
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project

Environmental Management Science Program Research in Colorado

National Renewable Energy Laboratory

54847-CO - Photocatalytic and Chemical Oxidation of Organic Compounds in Supercritical Carbon Dioxide

Year of Award: 1996 **Amount of Award:** $660,000
Problem Area: Mixed Waste
Science Category/SubCategory: Separations Chemistry / Catalyst Chemistry and Waste Treatment
Principal Investigator: Dr. Daniel M. Blake, 303-275-3702, blaked@tcplink.nrel.gov
Major Collaborator(s): Peter Hoekstra at Coleman Research Corporation
For More Information: http://www.doe.gov/em52/54847.html

Description Provided by Investigator:

The objective of the research is to develop new chemistry for the removal of organic contaminants from supercritical carbon dioxide. This has application in processes used for continuous cleaning and extraction of parts and waste materials. A secondary but very significant objective is to increase the fundamental understanding of photocatalytic chemistry. Cleaning and extraction using supercritical carbon dioxide ($scCO_2$) can be applied to the solution of a wide range of environmental and pollution prevention problems in the DOE complex. Work is being done that explores $scCO_2$ in applications ranging from cleaning contaminated soil to cleaning components constructed from plutonium. The rationale for use of $scCO_2$ are based on the benign nature, availability and low cost, attractive solvent properties, and energy efficient separation of the extracted solute from the solvent by moderate temperature or pressure changes. To date, R&D has focussed on the methods and applications of the extraction steps of the process. Little has been done that addresses methods to "polish" the $scCO_2$ for recycle in the cleaning or extraction operations. In many applications it will be desirable to reduce the level of contamination from that which would occur at steady state operation of a process. This research addresses chemistry to achieve that. This would be an alternative to removing a fraction of the contaminated $scCO_2$ for disposal and using makeup $scCO_2$. A chemical polishing operation can reduce the release of CO_2 from the process. It can also reduce the consumption of reagents that may be used in the process to enhance extraction and cleaning. A polishing operation will also reduce or avoid formation of an additional waste stream. Photocatalytic and other photochemical oxidation chemistry have not been investigated in $scCO_2$. The large base of information for these reactions in water, organic solvents, or air suggest that the chemistry will work in carbon dioxide. There are compelling reasons to believe that the properties of $scCO_2$ should increase the performance of photocatalytic chemistry over that found in more conventional fluid phases.

The objectives for this project are:

1) to determine if photocatalytic or other clean oxidation chemistry can be applied to the removal of organic or inorganic contaminants that are introduced into supercritical carbon dioxide during its use as an extraction and cleaning medium. The target will be contaminants left in solution after the bulk of solutes have been separated from the fluid phase by changing pressure and/or temperature (but not evaporating the CO_2). This is applicable to development of efficient separations and will strengthen pollution prevention strategies that eliminate hazardous solvents and cleaning agents.

2) to explore the use of supercritical carbon dioxide as a solvent for the photocatalytic oxidation of organic compounds and to compare it to other types of oxidation chemistry. This will add to the fundamental understanding of photocatalytic oxidation chemistry of particulate semiconductors and provide new knowledge about conditions that have relevance to the chemical fixation of carbon dioxide.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW03	C-287	Mixed Low Level Waste Project
+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
NV214	C-53	Industrial Sites
+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
RL-ER08	C-147	Groundwater Management
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Colorado

Colorado State University

55012-CO - Extraction and Recovery of Mercury and Lead from Aqueous Waste Streams Using Redox-active Layered Metal Chalcogenides

Year of Award: 1996 **Amount of Award:** $333,000
Problem Area: Mixed Waste
Science Category/SubCategory: Separations Chemistry / Ligand Design and Ion-exchange
Principal Investigator: Dr. Peter K. Dorhout, 970-491-0624, pkd@lamar.ColoState.EDU
For More Information: http://www.doe.gov/em52/55012.html

Description Provided by Investigator:

There are numerous practical reasons for selectively separating *heavy metal ions* of all types from aqueous media. A few obvious examples are the remediation of hazardous or radioactive waste, the remediation of contaminated groundwater, and the recovery of precious and/or toxic metals from industrial processing solutions. A variety of well-known techniques are available to the chemist or engineer for these tasks, including solvent extraction, ion-exchange chromatography, and precipitation. In modern applications of these techniques, *the recovery and re-use* of the extractant materials is becoming more and more important. This is being driven by tougher environmental regulations, the high initial costs of new, more effective, and more selective extractants, and the need to minimize the volume of waste destined for permanent disposal.

Many heavy metal ions are "soft" Lewis acids, which means that their affinity for soft donor atoms such as phosphorus and sulfur are considerably higher than for hard donor atoms such as nitrogen and oxygen. Examples of soft metal ions are Hg^{2+}, Pb^{2+}, Cd^{2+},Cu^{2+}, Ag^+, Au^{3+}, Pt^{4+}, and Tl^+. (Examples of hard metal ions include Li^+ and the other alkali metal ions, Mg^{2+} and the other alkaline earth metal ions, Ti^{4+}, and Cr^{3+}.) Many of the soft metal ions are of concern because they are highly toxic and are present in a variety of waste streams that can potentially contaminate the environment if released. For example, the following soft metal ions are currently identified for regulation under RCRA/SDWA: Cu^{2+}, Ag^+, Cd^{2+}, Hg^{2+}, Pb^{2+} and Tl^+. Safe, efficient, and cost effective separation *and recovery* of these metal ions from waste streams is therefore an important scientific and technological goal.

Contamination or potential contamination of surface waters and groundwater has already occurred in many locations, necessitating, as above, safe, efficient, and cost effective remediation in the very near future. For example, the Department of Energy must pre-treat, treat, and dispose of a number of aqueous high-level and mixed waste streams that contain mercury, lead, and/or other soft heavy metals. To satisfy *environmental concerns,* these soft, heavy elements must be removed from the waste (along with certain other heavy metals and radionuclides) before the bulk of the remaining waste can be disposed of in sub-surface vaults. As a particular case in point, there are currently 1.5 x 10^6 gallons of ICPP sodium-bearing waste in which $[H^+] \sim 1.5$ M, $[Hg^{2+}] \sim 0.002$ M, and $[Pb^{2+}] \sim 0.001$ M. Mercury is present in these streams because it was added to the acidic processing solutions to catalyze the dissolution of aluminum metal. Current technologies for the selective extraction of mercury and lead need to be improved or replaced for the following reasons: (i) *selectivity* for mercury and lead should be improved; (ii) *decontamination factors* should be increased; (iii) *recovery* of mercury and lead from the extractants should be required to allow for recycling and reuse of the extractants, lower costs, and minimization of the volume and mass of the final form of mercury and lead to be disposed of. All of these concerns will be addressed in our proposal.

Besides mercury- and lead-contaminated waste in the DOE complex, there are many other examples of anthropogenic or naturally-occurring soft-heavy-metal-ion pollution that are of significant environmental concern. For example, high concentrations of lead are found in soils in many U.S. urban areas. Lead must also be removed from contaminated wastes and soil at batteryrecycling Superfund sites. Both lead and copper contaminate soil at the Aberdeen Proving Ground in Maryland, and lead, copper, and cadmium are present in storm water runoffs entering Lakes Bay, New Jersey. Highly toxic thallium(I) is present in natural waters and wastewaters. Mercury, of course, is present in many aquatic environments, and the remediation of such environments, or the avoidance of contamination, is an area of active interest.

This research is also concerned with the design, synthesis, and evaluation of new redox active materials. These materials should be capable of being selective for softer cations, as described above, and express redox-active reversibility to enable recovery of the ions of interest; consequently, our synthetic paradigm focuses on the use of special building blocks. These chemically "soft" building blocks, such as sulfides and thiophosphates, are combined with redox actove metals, such as molybdenum, nickel, or cobalt, to create low-dimensional open-framework structures.

Although our research is concerned with removing soft heavy metal ions from *aqueous* solutions, our work is relevant to the extraction of these metal ions from contaminated soils. This is because soil remediation involves leaching the metal ions out of the soil and into aqueous solutions (e.g. acetic acid/sodium acetate or acidic potassium iodide). Clearly, a methodology for re-extracting the heavy metal ions from aqueous solution is a desirable goal.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§ RL-WM03	C-193	Solid Waste Storage and Disposal
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW03	C-287	Mixed Low Level Waste Project
+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ OR-48101	C-99	Offsite Remedial Action
+ OR-46301	C-107	Portsmouth Remedial Action
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
RL-ER08	C-147	Groundwater Management
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Delaware

University of Delaware

54661-DE - Electrochemical Processes for In-Situ Treatment of Contaminated Soils

Year of Award: 1996 **Amount of Award:** $317,000
Problem Area: Remedial Action
Science Category/SubCategory: Separations Chemistry / Catalyst Chemistry and Waste Treatment
Principal Investigator: Dr. Chin-Pao Huang, 302-831-8428, huang@ce.udel.edu
For More Information: http://www.doe.gov/em52/54661.html

Description Provided by Investigator:

This project will study electrochemical processes for the in situ treatment of soils contaminated by mixed wastes, i.e., organic and inorganic. Soil samples collected from selected DOE waste sites will be characterized for specific organic and metal contaminants and hydraulic permeability. The soil samples are then subject to desorption experiments under various physical-chemical conditions such as pH and the presence of surfactants. Batch electro-osmosis experiments will be conducted to study the transport of contaminants in the soil-water systems. Organic contaminants that are released from the soil substrate will be treated by an advanced oxidation process, i.e., electron-Fantan. Finally, laboratory reactor integrating the elector-osmosis and elector-Fatan processes will be used to study the treatment of contaminated soil in situ.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ AL007	C-7	Environmental Restoration
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV212	C-49	Underground Test Area (UGTA)
§ NV214	C-53	Industrial Sites
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER02	C-129	200 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in the District of Columbia

Naval Research Laboratory

55188-DC - Chemical Decomposition of High-Level Nuclear Waste Storage/Disposal Glasses Under Irradiation

Year of Award: 1996 **Amount of Award:** $489,000
Problem Area: High Level Waste
Science Category/SubCategory: Materials Science / Radiation Effects On Storage Materials
Principal Investigator: Dr. David L. Griscom, 202-404-7087, griscom@ccsalpha2.nrl.navy.mil
For More Information: http://www.doe.gov/em52/55188.html

Description Provided by Investigator:

The Offices of Energy Research and Environmental Management are immediately concerned with the development of storage/immobilization media for high-level nuclear wastes and excess weapons plutonium. These media must be stable and free of risk to the public or to the environment for a period of at least 200 years and, if possible, they should be suitable for much-longer-term local containment within geologic repositories. The storage media of choice at this moment are glassy forms, which can take on an enormously wide range of compositions, particularly if the various waste streams are to be vitrified with a minimum of (economically undesirable) pretreatments. Borosilicate glasses will be used for the initial vitrification of high-level nuclear wastes in the U.S. and Europe. Such glasses have been extensively tested for the effects of ionizing radiations on their durability against aqueous leaching. In general, α, β, γ, and α-recoil radiations are found to affect leach rates, though not to such a degree as to prevent these glasses from being employed as storage/immobilization media. Nevertheless, evidence of microbubble formation in such glasses has been noted during electron-beam irradiation in electron microscopes, and considerable (though still disputed) evidence has been given that bubble formation is greatly enhanced in glasses first exposed to γ rays or ion beams. It is widely supposed that these microbubbles contain oxygen molecules, though direct determinations of the gas contents of the bubbles have been lacking. If the bubbles are indeed due to oxygen molecules, it would be inferred that the glasses are decomposing into chemically reduced regions (perhaps, e.g., elemental metals) and free oxygen. This possibility is generally accepted with little alarm, since little or no effect on the leach rate has been shown to result. The guiding premise has been that the greatest threat to vitrified high-level nuclear wastes during the first 200 years (corresponding to the length of time before sealing of the geologic repository) is attack by ground water. Not considered in previous performance analyses has been the possibility that some of the metal-jacketed glass logs might not be attacked by ground water at all but instead may be left in their hermetically sealed steel canisters to radiolytically convert themselves into chemical explosives comprising flammable metals in a pure oxygen atmosphere. Note that the stored chemical energy of such a system would be far higher than the values determined by differential scanning calorimetry, an experiment which typically involves temperatures no higher than 700 C and does not measure or confine any evolved oxygen. Radiolytically decomposing high-level nuclear waste glasses sealed in steel canisters could conceivably become self-detonating due to electrical discharges associated with non-uniform irradiation or spontaneous fracturing of the vitreous medium. The hazards to the environment and to the public of such a scenario are obvious. Only the probability of occurrence is unknown. The present research effort is designed to:

(1) demonstrate unambiguously the nature(s) of any radiation-induced gas phases which may be dissolved in high-level-nuclear-waste-glass forms and lead to bubble formation,

(2) provide fundamental knowledge necessary to assess the vulnerability of these forms to chemical explosion, particularly if dissolved oxygen is verified, and

(3) develop an efficient method of surveying wide ranges of potential waste glass compositions to determine the dependence of radiolytic oxygen evolution on glass composition and hence determine compositions with superior resistance to decomposition.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§ ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§+ RL-TW08	C-185	Process Waste Privatization Infrastructure
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§ SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in the District of Columbia

Naval Research Laboratory

60141-DC - Gamma Ray Imaging for Environmental Remediation

Year of Award: 1997 **Amount of Award:** $780,000
Problem Area: Spent Nuclear Fuel
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Sensors and Techniques
Principal Investigator: Dr. W. Neil Johnson, 202-767-6817, johnson@osse.nrl.navy.mil
Major Collaborator(s): Dr. Paul N. Luke at Lawrence Berkeley National Laboratory
For More Information: http://www.doe.gov/em52/60141.html

Description Provided by Investigator:

The research is a three year development program to apply high resolution gamma-ray imaging technologies to environmental remediation of radioactive hazards. High resolution, position-sensitive germanium detectors are being developed at the Naval Research Laboratory for space applications with support from the Office of Naval Research and the National Aeronautics and Space Administration. In the program, we will model the performance of these detectors for direct imaging of spent nuclear fuels and fissile materials and Compton scatter imaging of large objects of arbitrary size, investigate fabrication of field-usable detectors, and demonstrate the performance of such a system using a small configuration of detectors.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Spent Nuclear Fuel problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Spent Nuclear Fuel".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
AL024	C-3	Grand Junction Office (GJO) All Other Projects
AL007	C-7	Environmental Restoration
+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
NV212	C-49	Underground Test Area (UGTA)
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
OR-43204	C-77	ORNL Bethel Valley Deactivation and Decommissioning
+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ OR-45301	C-103	Paducah Remedial Action
+ OR-46301	C-107	Portsmouth Remedial Action
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
RL-ER08	C-147	Groundwater Management
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW04	C-169	Retrieval Project
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project
+ SR-HL02	C-253	F-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations

Environmental Management Science Program Research in the District of Columbia

Georgetown University

54716-DC - Polyoxometalates for Radioactive Waste Treatment

Year of Award: 1996 **Amount of Award:** $333,000
Problem Area: High Level Waste
Science Category/SubCategory: Separations Chemistry / Ligand Design and Ion-exchange
Principal Investigator: Dr. Michael T. Pope, 202-687-6073, POPE@GUVAX.ACC.GEORGETOWN.EDU
Major Collaborator(s): Jeffrey Bryan at Oak Ridge National Laboratory
For More Information: http://www.doe.gov/em52/54716.html

Description Provided by Investigator:

Environmental Restoration of Nuclear Sites

The legacy of fifty years of nuclear processing for weapons and power production is a staggering environmental problem. In the U.S. alone there are more than 100 contaminated installations in 36 states and territories, and similar situations exist in other countries. The costs of cleanup using current technologies have been estimated to be in excess of $100B. Defense waste accounts for 95% of the *volume* of the total U.S. radioactive waste, but 90% of the *activity* is contained in spent commercial nuclear fuel. The most serious challenge in terms of environmental restoration is provided by the tank wastes at the DOE Hanford site. Most of this waste is stored in *ca* 60 underground tanks each holding a million gallons of alkaline slurry. The chemical compositions of the tank wastes are highly complex and are in many cases unknown in detail, since waste streams from several fuel-processing operations were combined, together with residues from many other secondary processes. Acidic waste streams were treated with sodium hydroxide to minimize tank corrosion, making the wastes highly concentrated in non-radioactive sodium salts. The tanks are known to contain significant concentrations of *ca* 50 elements and a range of organic species (solvents and sequestrants). The radioactive elements present that are of most concern from the viewpoint of toxicity levels, are Sr, Tc, Cs, U, Pu and other transuranics. Other radioactive species include Y, I, Ce, Pm and Eu. All of the components of the wastes are distributed between insoluble sludge, a high ionic strength aqueous supernatant, and a soluble salt cake crystallized from the supernatant.

Three phases of processing have generally been considered for waste treatment: (a) pretreatment of raw tank waste for subsequent separations; (b) phvsical or chemical separations; (c) solidification (usually vitrification) of high level waste (HLW) for subsequent deep geologic storage. Although several potential processes have been described, serious difficulties and limitations remain. These include the distribution of radioactive components between the supernatant, salt cake, and sludge; the difficulties inherent in handling possible colloidal dispersions of sludge particles; and the incomplete characterization of the chemical species present. Thus, although it might be expected that lanthanide (Ln) and actinide (An) species would be present in the insoluble sludge, since the solutions are highly alkaline, the presence of organic species including sequestrants such as EDTA and nitrilotriacetic acid in some of the tanks may result in partial solubilization.

This research addresses the questions of separating and concentrating radioactive components of tank wastes, especially lanthanide (Ln) and actinide (An) species, and technetium. It is known that such radioactive isotopes constitute less than one part in 10^4 of the mass present in most tanks, so that if efficient separations can be devised, the total volume of high level wastes (HLW) to be stored is reduced to more manageable quantities. Three project areas will be pursued concurrently: (a) Development of known robust polyoxometalate cryptands for selectively binding lanthanides (Ln) and actinides (An). Selectivity is based upon cation charge and size; approximate polyoxometalates discriminate against most nonradioactive components of the tank wastes. (b) Incorporation of technetium into stable, non-volatile polyoxometalate complexes for subsequent separation and immobilization. (c) Conversion of polyoxometalates under relatively mild conditions to inert tungsten bronze-like materials that incorporate the radioactive waste cations and which could be used as alternative waste forms. Research at Georgetown University will be carried out using on-radioactive isotopes or those like ^{238}U that present low radiological hazards. Project (b) will be initiated using rhenium as a surrogate for technetium in view of the established similarities of these elements in polyoxometalates. Collaborative arrangements with Oak Ridge National

Laboratory will allow optimized procedures developed at Georgetown to be extended to the transuranic elements, technetium, and simulated tank wastes.

A Brief Introduction to Polyoxometalates and Polyoxometalate Chemistry

The complexes known as polyoxometalates (POMs, heteropolyanions) form a class that is of *unsurpassed structural and electronic variety and versatility* in inorganic and organometallic chemistry. These substances are discrete molecular-ionic species with the general formula $[X_xM_mO_y]^{n-}$ ($m > x$), where the addenda atoms, M, typically are V^V, Nb^V, Mo^{VI}, W^{VI}; and the heteroatoms, X, can be one or more of *ca* 70 other elements in a variety of oxidation states. Salts and free acids of POM anions are water- and organic-solvent-soluble and generally have high thermal stabilities (*ca* 500°C). The anions may contain 30 or more metal atoms (the current record is a discrete water-soluble species with 154 molybdenum atoms!), and the salts frequently have molecular weights exceeding 10,000.

POMs have many important applications: they are industrial acid- and redox catalysts (propene hydration, oxidation of methacrolein, etc.) and they find use in analytical and clinical chemistry, medicine (antiviral and antitumoral agents, electron-dense imaging agents), materials science (electronic and protonic conductors), and as selective and high-capacity oxidants and reductants. Their properties and structures are well-suited to examining and modelling theories and mechanisms in areas as diverse as electron transfer, mixed valence chemistry, topology, host-guest and cryptate chemistry, self-assembly and template processes, small molecule activation, polymetallic centers in bioinorganic chemistry, cooperative magnetic behavior, surface science, heterogeneous catalysis, geology, etc.

Polyoxometalates are most commonly formed in aqueous or polar nonaqueous solutions by acid-base condensation-addition processes, e.g.

$$12\ MoO_4^{2-} + HPO_4^{2-} + 23\ H^+ \dashrightarrow [PMo_{12}O_{40}]^{3-} + 12\ H_2O$$

or by hydrothermal methods. The resulting anions are isolated as salts or free acids and are stable in solution over a pH range that is characteristic of the particular anion. The structures are based most often on arrangements of edge- and comer-shared MO_6 octahedra. and, for reasons of clarity, are frequently illustrated in this fashion.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ RL-TW05	C-173	Process Waste Support
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
§ SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Florida

Florida State University

54893-FL - Research Program to Determine Redox Properties and Their Effects on Speciation and Mobility of Pu in DOE Wastes

Year of Award: 1996 **Amount of Award:** $875,000
Problem Area: Remedial Action
Science Category/SubCategory: Actinide Chemistry / Actinide (Heavy Element) Chemistry
Principal Investigator: Dr. Gregory R. Choppin, 904-644-3875, CHOPPIN@CHEM.FSU.EDU
Major Collaborator(s): Dr. Dhanpat Rai at Pacific Northwest National Laboratory
For More Information: http://www.doe.gov/em52/54893.html

Description Provided by Investigator:

Plutonium contamination is a major problem at many DOE sites. This research seeks to provide fundamental data and models for predicting plutonium speciation and environmental behavior which will allow evaluation of the many processes proposed for remediation of plutonium-containing DOE wastes. Basic to this prediction are: 1) the complete fundamental data on aqueous complexation, solubility reactions, and geochemical conditions under which different plutonium oxidation states transform from one to another; and 2) a model containing this fundamental data which can predict site-specific reactions. We propose to summarize existing data and develop additional fundamental data to measure the oxidation state (or states) in a variety of solid/solution systems in the presence and absence of chemicals likely to be pre sent in DOE wastes of environmental systems and which can promote redox transformations and complexation reactions. Specifically, we will 1) determine stability constants of Pu(IV) with strong complexants such as EDTA and DTPA,2) determine the geochemical conditions under which different reductants (e.g., Fe(0), Fe^{2+}, Fe(II)-containing solids, and humics) can reduce Pu(VI) to Pu(III)/Pu(IV) and oxidants (e.g., MnO_2 and radiolytic products) that can oxidize Pu(IV) to Pu(V)/Pu(VI), and 3)summarize fundamental data into a model and test the accuracy of this model in a limited set of conditions using plutonium contaminated sediments or sediments spiked with different oxidation states. The principle investigator has many years of plutonium research experience and have all the necessary knowledge and facilities to carry out this research. The main output from this project will be the data and the model to reliably predict the plutonium oxidation states, transformation reactions, and plutonium behavior in diverse geologic environments and to allow the development of appropriate new technologies or evaluate the effectiveness of proposed technologies.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ AL024	C-3	Grand Junction Office (GJO) All Other Projects
§ NV214	C-53	Industrial Sites
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ OR-48101	C-99	Offsite Remedial Action
§+ OR-45301	C-103	Paducah Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER02	C-129	200 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ RF014	C-213	Industrial Zone Closure Project
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
ID-HLW-101	C-29	High-Level Waste Pretreatment
ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
+ RL-TP07	C-161	Plutonium Finishing Plant (PFP) Vault Management
+ RL-TW05	C-173	Process Waste Support
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
+ RL-TW08	C-185	Process Waste Privatization Infrastructure
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
+ SR-HL01	C-249	H-Tank Farm
SR-HL05	C-265	Vitrification
+ SR-SW01	C-281	Consolidated Incinerator Facility
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in Florida

University of Florida

54982-FL - Analysis of Surface Leaching Processes in Vitrified High-Level Nuclear Wastes Using In-Situ Raman Imaging and Atomistic Modeling

Year of Award: 1996 **Amount of Award:** $559,000
Problem Area: High Level Waste
Science Category/SubCategory: Materials Science / Chemical and Structural Properties Of Storage Materials
Principal Investigator: Dr. Joseph H. Simmons, 352-392-6679, SIMMONS@QUARTZ.MSE.UFL.EDU
For More Information: http://www.doe.gov/em52/54982.html

Description Provided by Investigator:

The research proposed combines a novel investigative technique with novel modeling studies to analyze leaching processes in glasses. Its utility is that it will provide both a means of conducting fundamental studies of the corrosion behavior of high valence and multivalent ions in the waste glass as well as a proven *in-situ* method for monitoring the chemical corrosion behavior of radioactive waste glasses, remotely and in burial sites. The research has three major thrusts: (1) the development of *in-situ* Raman Imaging Spectroscopy for a detailed examination of leaching processes and associated structural changes and mineral precipitates on the surface of borosilicate glasses loaded with simulated high-level nuclear wastes, (2) the application of this method to the analysis of transition states and their energetics during surface leaching by novel modeling studies, and by comparison with existing methods of IR, Auger XPS and SIMS spectroscopy, SEM, TEM and STM/AFM microscopy and BET surface analysis, and (3) the extension of *in-situ* Raman Imaging Spectroscopy for conducting remote tests on radioactive loaded samples, and for the examination of variations over the surface of large ingots. The research comprises fundamental studies of (1) the relationship between leaching processes and Raman spectroscopy, using both tests on simple liquids and quantum mechanical modeling, and (2) the examination of transition states in hydration processes involving the higher valence and multivalent ions and their use in predicting, with high accuracy, their solubility in aqueous solutions using both experimental and quantum mechanical modeling methods. The combination of these two studies has the potential to offer a novel method which has both *in-situ* and remote capabilities for the analysis of leaching processes on high-level radioactive waste glasses. This method makes possible tests on radioactive materials with greatly reduced personnel exposure, and makes possible the examination of leaching processes in real-time in burial sites. Finally, this method can be applied to the continuous monitoring of the conditions of glass boules during actual disposal conditions.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

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Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§ ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ RL-TW08	C-185	Process Waste Privatization Infrastructure
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
§ SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Georgia

Georgia Institute of Technology

54807-GA - Studies Related to Chemical Mechanisms of Gas Formation in Hanford High-Level Nuclear Wastes

Year of Award: 1996 **Amount of Award:** $320,000
Problem Area: High Level Waste
Science Category/SubCategory: Inorganic Chemistry / Multiphase/Gaseous Chemistry
Principal Investigator: Dr. E. Kent Barefield, 404-894-4034, kent.barefield@chemistry.gatech.edu
For More Information: http://www.doe.gov/em52/54807.html

Description Provided by Investigator:

The research has its origin in studies at Georgia Tech into the chemical (as opposed to radiolytic) mechanisms of gas formation (H_2, N_2O, N_2, and NH_3) in nuclear waste storage tanks at Hanford, Washington, which has been supported since 1991 under DOE's comprehensive Flammable Gas Safety Program. That gas was generated in certain of the Hanford waste storage tanks was recognized in the late 1970's, but the magnitude of the problem was not apparent until a decade or so later when several waste tanks were fitted with monitoring devices to determine the identity and amounts of the gases produced. Even then it was not until early 1993 that the amount of ammonia was quantitated.

There are many types of waste in the 177 underground storage tanks at Hanford, but the tanks that evolve gases all contain large amounts of NO_3^-, OH^-, $Al(OH)_4^-$and NO_2^-, and varying amounts of organics, including some common metal chelating agents. Wastes are heterogeneous and consist of a layer of sediment (non-convective layer) and a highly concentrated supernatant (convective layer). The first three ingredients and some of the organics arise directly from the plutonium production process, which involves dissolution of aluminum clad fuel elements in concentrated nitric acid, solvent extraction of plutonium and uranium, and basification of the actinide-depleted liquor with sodium hydroxide to allow for storage in carbon steel tanks. The introduction of metal chelating agents, including citrate, glycolate, EDTA, and HEDTA (N-2-hydroxyethylethylenediaminetriacetic acid) resulted from various campaigns to reduce the levels of fission products by secondary separation processes. Nitrite is produced from NO_3^- by radiolytic processes.

Although many of the boundary conditions that affect gas production, and certain details of the mechanism have been elucidated, many fundamental questions remain that ultimately bear on the processing of these wastes. For example, prediction of the combustion hazard depends upon both the knowledge of the composition of the waste and the nature of the thermal and radiolytic decomposition of the constituents. From our work on the mechanism of thermal production of gases in simulated waste mixtures using HEDTA (N-hydroxy ethylethylenediaminetriacetic acid), some of its fragmentation products, and glycolate as models we have identified several mechanistic issues that must be addressed to support engineering of large scale waste processing. Although only funding for research at Georgia Tech is requested, we expect that this work will be done in collaboration/consultation with scientists at DOE facilities with whom we have worked closely over the past five years, *vide infra.*

In early, elegant work Delegard studied reactions in simulated waste slurries to show that aluminate, NO_2^- and/or NO_3^-, and a chelating agent such as glycolate or HEDTA were necessary for gas production. ED3A (ethylenediaminetriacetic acid) and oxalate were found as products of HEDTA degradation and oxalate as a product of glycolate degradation. EDTA did not produce gas under any conditions. The mechanistic interpretation of these data centered around possible binding of the chelating agent prior to reaction with the oxidant, but did not consider how thiscomplex reacted with the oxidant(s) or mechanistic pathways leading to the individual gases.

During the past five years we have utilized product identification and kinetic analysis in an attempt develop mechanistic models for the thermal generation of the volatile products H_2, N_2, N_2O, and NH_3 and a variety of condensed phase products including formate and oxalate in homogeneous waste simultants. The simulant consists of 0.21 M organic chelating agent (i.e.HEDTA, glycolate), 2.5 M sodium nitrite, 2.2 M sodium nitrate, 2.0 M sodium hydroxide, and 1.5 M sodium aluminate. The following narrative describes the postulated mechanistic sequence for the thermal degradation of HEDTA to ED3A and the supporting experimental observations. Unlike Delegard's mechanism ours does not involve binding of aluminum by the chelating agent.

In experiments dealing with the thermal degradation of HEDTA to ED3A we have observed that

- no reaction takes place in the absence of aluminate

- the concentration of NO_2^- decreases with time

- the concentration of NO_3^- remains constant throughout the course of reaction

- use of ^{15}N-labeled reagents indicates that NO_2^- is the source of nitrogen for N_2O and N_2 and the bulk of the NH_3 (a small amount is derived from nitrogen- containing substrates such as HEDTA).

The initial step of our postulated mechanism for the reaction of HEDTA or of glycolate involves the generation of the nitrite ester of the hydroxyl group in either molecule. Support for this as the initial reaction comes from the results of the thermal decomposition of the nitrite ester of methyl glycolate produced by the exchange reaction of methyl glycolate and tert-butyl nitrite. Thermolysis of this nitrite ester in aqueous base produced H_2, N_2O, formate and oxalate. The odor of ammonia was clearly present but a quantitative determination of this product was not undertaken, nor was any analysis done for N_2. The mechanistic sequence shown in Scheme 1 accounts for the production of formate and oxalate. The formation of H_2 and the nitrogen products will be considered later.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

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Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§ ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
§+ RL-TW04	C-169	Retrieval Project
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§+ RL-TW08	C-185	Process Waste Privatization Infrastructure
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
§ SR-HL05	C-265	Vitrification
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in Georgia

Georgia Institute of Technology

55042-GA - Quantifying Silica Reactivity in Subsurface Environments: Controls of Reaction Affinity and Solute Matrix on Quartz and SiO2 Glass Dissolution Kinetics

Year of Award: 1996 **Amount of Award:** $358,994
Problem Area: High Level Waste
Science Category/SubCategory: Geochemistry / Sorption/Desorption
Principal Investigator: Dr. Patricia M. Dove, 404-894-6043, patricia.dove@eas.gatech.edu
For More Information: http://www.doe.gov/em52/55042.html

Description Provided by Investigator:

An immediate goal of this OER/OEM initiative is the development of a predictive framework of kinetic data for mineral-solution reactions that accurately describes the current and future behavior of earth systems. Reaction rates and mechanisms are essential elements in deciphering mineral/material reactivity trends within compositional series or across a matrix of complex solution compositions. The goal of the research addresses this gap in our current understanding by quantifying the reactivity of crystalline and amorphous SiO_2 phases in the complex fluids of natural systems.

There are a number of important motivations for quantifying SiO_2 reactivity in the fluids of subsurface environments. First, quartz and silica glass are the compositional end-member crystalline and amorphous oxides to the large classes of silicate minerals and glasses. Second, an understanding of fundamental controls on the reactivity of simple SiÑO bonded phases establishes baseline behavior for silica phases widely found in waste storage environments and the host rock silicate minerals. These minerals comprise >90% of the earth's crust and dominate virtually every repository rock-water system. Third, complex silicate glasses will be the front line of defense in containing radioactive wastes in both interim and long-term storage strategies. However, we have little quantitative understanding of pure SiO_2 reactivity in the solutes of natural and perturbed groundwaters even though current EM strategy calls for dispersal of waste into silica-based glass materials.

Recent studies show that simple solutes, sodium and potassium significantly enhance the reactivity of silica minerals and that this salt effect has a complex pH-dependence. However, the effect of other solutes frequently found in groundwater and soil solutions in pristine or contaminated areas is poorly understood. Further, there is presently little quantitative knowledge of how reaction affinity modifies this solute dependence. Both of these issues are important because the available data suggest that solutes and reaction affinity exert complex rate enhancing as well as rate inhibiting effects. Given the experience and publication record of the P.I. in the geochemical kinetics of mineral-water interactions, the research is a cost-effective approach to advancing our basic and applied scientific knowledge of solute controls on silica reactivity in natural and engineered Earth Systems.

Using an experimental approach which integrates techniques from surface science and geochemical kinetics, this study will measure the dissolution rate of quartz and silica glass in a series of single and mixed solute solutions over a range of variable pH and temperature. Rates will be measured over a range of reaction affinities by adjusting the steady state silica concentration produced during the dissolution reactions. These data will allow us to construct a comprehensive quantitative model of solute controls on the reactivity of crystalline and glassy SiO_2. The kinetic portion of the study will be conducted in parallel with in situ and ex situ surface sensitive analyses of selected samples/conditions. Findings will establish quantitative relationships between silica reactivity and a number of solution chemistries which have never been investigated or are presently understood in only a qualitative sense. Further, they will allow us to test the hypothesis that the solvation properties of dissolved species govern silica reactivity in a systematic and predictable way. If valid, we may be able to develop a powerful predictive tool for accurately estimating the influence of complex solute chemistries found in subsurface environments on silica reactivity and durability.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

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Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§ ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ RL-TW08	C-185	Process Waste Privatization Infrastructure
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§ SR-HL05	C-265	Vitrification
AL007	C-7	Environmental Restoration
+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
NV212	C-49	Underground Test Area (UGTA)
NV214	C-53	Industrial Sites
+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Georgia

Georgia Institute of Technology

55218-GA - Seismic Surface-Wave Tomography of Waste Sites

Year of Award: 1996 **Amount of Award:** $358,202
Problem Area: Remedial Action
Science Category/SubCategory: Geophysics / Subsurface Imaging
Principal Investigator: Dr. Timothy L. Long, 404-894-2068, tim@namazu.eas.gatech.edu
Major Collaborator(s): William Doll at Oak Ridge National Laboratory
For More Information: http://www.doe.gov/em52/55218.html

Description Provided by Investigator:

Studies of the earth using surface waves are extensive. The early targets were crustal thickness and upper mantle structure because surface waves are well recorded on the early long period instrumentation and because the velocity contrast between the crust and mantle exhibits pronounced dispersion. When simple (as in flat layered) earth models are employed, the vertical variations in velocity associated with differing crustal structures can be obtained by using analytical techniques for computing dispersion relations. However, the more interesting variations in surface structure, those related to major geologic structures, represent lateral variations in material properties. Simple analytical solutions to the elastic wave equation do not exist for media with lateral heterogeneities and/or irregular geometries. Thus, for complex structures, interpretations have had to wait for practical numerical solutions and more advanced computational facilities. For these reasons, perhaps, the application of surface waves to shallow engineering problems has been slow.

Surface wave dispersion methods have been attempted in seismic reflection to constrain the corrections for time delays introduced by variations in near surface velocity structure. The difficulties and mixed results in defining these "static" corrections include variations in the ratio of P to S wave velocities, expressed as Poisson's ratio, and the significant differences in computational methods applied to surface wave dispersion and reflection data. In soils engineering, the spectral analysis of surface waves (SASW) has been developed for determining the pavement strength of road beds and liquefaction potential of soils. The SASW technique is based on surface measurements of phase velocity above a structure which is assumed to consist of flat layers. In this work, we propose to extend the spectral analysis techniques to a tomographic inversion for group velocity and develop computer programs that will allow analysis at near real time in the field. More importantly, we propose research on techniques that will include lateral variation in structures.

The near surface can have a highly heterogeneous velocity structure. The velocity contrast between the soil layers and the unweathered rock can approach two orders of magnitude, when, in comparison, conventional reflection and refraction studies consider a 10 percent contrast very significant. Surface wave dispersion is sensitive to the depth and lateral variation in velocity contrasts of this high magnitude and thus are appropriate for examining the near surface. Typically, they are most sensitive to the shallowest layers and can complement refraction and reflection data which are more appropriate for deeper structures. In general, zones of soil and rock disturbances which have widths similar to or greater than their depths are ideal for detection by surface wave dispersion. These include trenches filled with debris, walled bunkers, and accumulations of liquid waste in depressed zones.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

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"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV212	C-49	Underground Test Area (UGTA)
§ NV214	C-53	Industrial Sites
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER02	C-129	200 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
+ RL-TW04	C-169	Retrieval Project
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
+ SR-HL02	C-253	F-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations

Environmental Management Science Program Research in Georgia

University of Georgia

54837-GA - Phytoremediation of Ionic and Methyl Mercury Pollution

Year of Award: 1996 **Amount of Award:** $825,485
Problem Area: Remedial Action
Science Category/SubCategory: Plant Science / Plant Genetics
Principal Investigator: Dr. Richard B. Meagher, 706-542-5925, meagher@bscr.uga.edu
For More Information: http://www.doe.gov/em52/54837.html

Description Provided by Investigator:

The long-term goal is to manipulate single-gene traits into plants, enabling them to process heavy metals and remediate heavy metal pollution by resistance, sequestration, removal, and management of these contaminants. We have successfully engineered a small model plant, Arabidopsis thaliana, to use a highly modified bacterial mercuric ion reductase gene, merA9, to detoxify ionic mercury (Hg^{++}), reducing it to Hg^{o}. Seeds from these plants germinate, grow, and set seed at normal growth rates on levels of Hg^{++} that are lethal to normal plants. A more serious problem is the methyl mercury produced by native bacteria at these sites, since it is concentrated up the food chain and poses the most immediate health threat to wildlife and humans. We propose that transgenic plants expressing both the bacterial organo mercury lyase (meB) and the mercuric ion reductase gene (mera) will a) remove the mercury from polluted sites and b) prevent methyl mercury from entering the food chain. It is also proposed that as soluble mercury vapor is transpired, it will be reoxidized and trapped in above ground tissues of the plant. These hypotheses will be tested first in model Plants and then in transgenic Yellow poplar, sweetgum, rice, and Spartina.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ NV212	C-49	Underground Test Area (UGTA)
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ OR-48101	C-99	Offsite Remedial Action

Environmental Management Science Program Research in Idaho

Idaho National Engineering and Environmental Laboratory

55416-ID - Control of Biologically Active Degradation Zones by Vertical Heterogeneity: Applications in Fractured Media

Year of Award: 1996 **Amount of Award:** $2,000,000
Problem Area: Remedial Action
Science Category/SubCategory: Microbial Science / Microbial Transport
Principal Investigator: Dr. Frederick (Rick) S. Colwell, 208-526-0097, fxc@inel.gov
Major Collaborator(s): James McKinley at Idaho National Engineering and Environmental Laboratory
Robert Smith at Idaho National Engineering and Environmental Laboratory
James Fredrickson at Pacific Northwest National Laboratory
T.C. Onstott at Princeton University
A. Reysenbach at the Rutgers, the State University of New Jersey
For More Information: http://www.doe.gov/em52/55416.html

Description Provided by Investigator:

The U.S. Department of Energy (DOE) is faced with cleaning up wastes from reactor and weapons production activities during the latter half of this century. Many DOE sites have contaminants that are difficult to access due to depth and complex geology and are challenging to degrade using conventional methods. Fundamental, field-based research is required to understand what is needed to address complex cleanup issues such as those that exist in fracture flow environments. **The key objective of this research is to determine the distribution of biologically active contaminant degradation zones in a fractured, subsurface medium with respect to vertical heterogeneities.** The research will be performed on samples collected from the Test Area North (TAN) site at the Idaho National Engineering Laboratory (INEL) where a dissolved trichloroethylene (TCE) plume is migrating in the Snake River Plain aquifer. To determine whether microbial degradation is spatially correlated to preferred flow paths for the contaminant and required electron donors and acceptors we will characterize the biological and abiological properties of cores and samples from multi-level samplers placed in the same borehole. We will use a combination of traditional microbiological methods (e.g., enrichments) and molecular tools to characterize the indigenous microbial communities. Collaboration with other EMSP investigators studying this site and the DOE Office of Environmental Management (EM40) which is implementing remediation will lead to more complete understanding of the biotic and abiotic processes in the subsurface at TAN. We believe that the fundamental research proposed will explain the distribution of microorganisms that can degrade TCE in the context of the geochemical and physical constraints under which these organisms function. This in turn will allow better decisions to be made with regards to the use of remedial technologies such as natural attenuation and in situ bioremediation at this geologically complex site.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§ RL-ER08	C-147	Groundwater Management
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Idaho

Idaho National Engineering and Environmental Laboratory

60424-ID - High Temperature Condensed Phase Mass Spectrometric Analysis

Year of Award: 1997 **Amount of Award:** $680,000
Problem Area: High Level Waste
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Mass Spectrometry
Principal Investigator: Dr. James E. Delmore, 208-526-2820, jed2@inel.gov
For More Information: http://www.doe.gov/em52/60424.html

Description Provided by Investigator:

Our current studies with high temperature ion emitting materials have demonstrated a significant lack of methods for determining chemical species in condensed phase materials in general, and at elevated temperatures in particular. We have developed several new research techniques for approaching this issue of high temperature chemical speciation, but new instrumentation is needed in order to more completely address the research needs. It is proposed to develop a new ultra high vacuum mass spectrometer system which combines the features of static and dynamic SIMS, surface ionization, and electron impact ionization of evaporating neutrals, in which miniaturized samples can be studied from room temperature up to 1500°C. All data will be collected from the same sample by rapidly interlacing the different ionization modes, which will significantly expedite data correlation. This proposed instrument will enhance research efforts in understanding chemical reactions and materials at high temperatures. Ongoing reserach at the INEEL in ion emitter studies will greatly benefit from this work, but benefits across a wide range of other fields can also be expected. An issue of significant interest to DOE waste management is that of the chemical stability of waste storage forms. These solid materials, primarily glasses, will be produced at high temperatures, then cooled and put into storage. The possibility exists that in a geologic repository heating from radioactive decay, combined with limited cooling, could result in extended storage at elevated temperatures. The studies that can be conducted with the proposed instrumentation can be applied to a wide range of high temperature processes and materials, and will add a new and needed dimension to the study of waste storage glasses, providing insights on the mobility and chemical speciation of the hazardous components.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

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Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§ ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
§+ RL-TW04	C-169	Retrieval Project
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
§ SR-HL05	C-265	Vitrification
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
NV214	C-53	Industrial Sites
+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER06	C-141	Decontamination and Decommissioning
RL-TP10	C-163	Accelerated Deactivation
RF014	C-213	Industrial Zone Closure Project
+ SR-SW01	C-281	Consolidated Incinerator Facility

Environmental Management Science Program Research in Idaho

University of Idaho

60144-ID - Flow Visualization of Forced and Natural Convection in Internal Cavities

Year of Award: 1997 **Amount of Award:** $1,077,000
Problem Area: Spent Nuclear Fuel
Science Category/SubCategory: Engineering Science / Design, Process and Modeling
Principal Investigator: Dr. John C. Crepeau, 208-526-5514, stf1004@decit.if.uidaho.edu
Major Collaborator(s): Randy Clarksean at Clarksean Associates
Donald M. McEligot at Idaho National Engineering and Environmental Laboratory
Yann G. Guezennec at Ohio State University
For More Information: http://www.doe.gov/em52/60144.html

Description Provided by Investigator:

This research project will focus efforts on developing techniques to model fluid flow in spent nuclear fuel canisters. One treatment technique is to inject gases which react with spent fuels into storage canisters, preventing the occurrence of pyrophoric reactions. The primary goals of this research are as follows: first, develop a method to visualize flow in the presence of a reacting surface; second, use the Matched-Index-of-Refraction facility at the INEEL in conjunction with laser doppler velocimetry to measure flow field velocities within a spent fuel canister; third, develop a computer model of the flow field and use the experimental results to validate the code.

Complex fluid flow in internal geometries occur in many engineering applications, including shell and tube heat exchangers, radiators, refrigeration systems and in drying canisters of spent nuclear fuel. When a nuclear fuel rod has reached the end of its useful life, it is removed from the reactor and placed in a cooling pool. Most of the fuel stored underwater has corroded and silt has deposited on and between the plates. The fuel needs to be prepared for long-term storage and the elements must be dried out. When corroded elements are exposed to air, dangerous pyrophoric reactions can occur. One method of preventing a pyrophoric reaction during drying is to introduce into the chamber an inert gas mixed with a small amount of oxygen to passivate the exposed fuel. This process forms an oxide layer which protects the fuel and prevents a pyrophoric reaction; however, this treatment process is poorly understood. We propose to investigate novel techniques of visualizing flow with surface reaction and flow in and around tube bundles, and combine the experimental results with computational models to fully characterize the flow field.

The University of Idaho (UI) will head the research effort and investigate flow visualization with surface reaction. Typical flow visualization techniques introduce bubbles or particles into a flow and observe their behavior as they move past a body. Flow with surface reaction reduces the concentration of particles in the overall flow. A new technique the UI will investigate uses magnetic particles suspended in oil as tracers, to represent oxygen, and a magnet to represent the fuel rod. Another technique uses fluorescent oxidizing particles as tracers. These experiments will visualize flow with surface reaction.

The Idaho National Engineering and Environmental Laboratory (INEEL) will utilize its state-of-the-art Matched-Index-of-Refraction (MIR) flow facility to investigate and visualize the flow throughout the drying chamber. Since many fuel rods are packed into the drying chamber, it is difficult to visualize the flow between the rods. The MIR technique allows observation of the fluid motion between the fuel rods and identifies areas of stagnant fluid in the chamber. The results from analyzing the flow with this method will allow safer and more efficient means of drying and passivating stored spent fuels.

In order to expedite the flow field analysis, Clarksean and Associates will perform computational fluid dynamics studies. Information from the flow with surface reaction analysis and the MIR experiments will be used to verify computational codes. These codes can then be used as an engineering tool to improve the design of fuel drying chambers and for the simulation of other drying methods. Further, these computational codes can form the foundation for studies and development efforts in other fields and industries where complex flows in internal geometries occur.

The research effort will benefit the Environmental Management Science Program (EMSP) in several ways. Visualization of flow with surface reaction in complex internal geometries is an area where little basic research has been performed. In addition to helping the DOE improve methods of treating spent nuclear fuels, the methods outlined here can improve our knowledge of many other engineering configurations. Doing a visualization study on this type of flow will allow determination of optimal fuel stacking geometries in a drying chamber, location of dead spaces in the flow field, and verification that the exposed fuel is properly passivated. Combining the experimental results with the computational models will provide a needed foundation and method for improving the treatment of spent nuclear fuel.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Spent Nuclear Fuel problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Spent Nuclear Fuel".

Environmental Management Science Program Research in Illinois

Argonne National Laboratory

55229-IL - The NOx System in Nuclear Waste

Year of Award: 1996 **Amount of Award:** $1,200,833
Problem Area: High Level Waste
Science Category/SubCategory: Inorganic Chemistry / Solid/Solution Chemistry
Principal Investigator: Dr. Dan Meisel, 630-252-3472, dani@anl.gov
Major Collaborator(s): Don Camaioni at Pacific Northwest National Laboratory
Thom Orlando at Pacific Northwest National Laboratory
For More Information: http://www.doe.gov/em52/55229.html

Description Provided by Investigator:

A collaborative program between ANL and PNNL is proposed to study the radiation, and radiation induced, chemistry of the NO_x system in waste simulants. The study will develop a computer model providing predictive capabilities for future EM operations including the characterization and pretreatment efforts. Essentially all of the chemistry that takes place in underground storage tanks is initiated by the little understood radiolytic effects on the concentrated nitrite/nitrate systems and its interaction with organic components of the waste. The ANL effort will develop quantitative data base of the dynamics of the early processes following the deposition of energy in the waste. The PNNL effort will focus on the interaction of NO_x with the organic components at slower time scales, and on identification of final products. The substrate systems will be complexants, paraffins, organic phosphates, phenylborates and their degradation products, all of which are of specific safety concern at various EM sites. The quantitative rate and yield data, and the mechanistic information from both efforts will be incorporated into a unified computer code that describes the chemical consequences of a variety of EM scenarios.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

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Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§+ RL-TW04	C-169	Retrieval Project
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations

Environmental Management Science Program Research in Illinois

Argonne National Laboratory

55247-IL - Sensors Using Molecular Recognition in Luminescent, Conductive Polymers

Year of Award: 1996 **Amount of Award:** $1,500,000
Problem Area: Mixed Waste
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Sensors and Techniques
Principal Investigator: Dr. Michael R. Wasielewski, 630-252-3570, wasielewski@anlchm.chm.anl.gov
Major Collaborator(s): David Walt at Tufts University
Kenneth Raymond at the University of California at Berkeley
For More Information: http://www.doe.gov/em52/55247.html

Description Provided by Investigator:

This program integrates three individual, highly interactive projects that will use molecular recognition strategies to develop sensor technology based on luminescent, conductive polymers that contain sites for binding specific molecules or ions in the presence of related molecules or ions. Selective binding of a particular molecule or ion of interest to these polymers will result in a large change in their luminescence and/or conductivity, which can be used to quantitatively sense the presence of the bound molecules or ions. Molecular recognition sites for a variety of toxic metals and organics will be developed. These include transition metals, heavy metals such as lead, uranium, and plutonium, as well as toxic organics, such as chlorinated and nitrated aromatic molecules. Research problems that will be addressed include: 1) designing molecular recognition sites that are highly selective for the ions and/or molecules of interest in the presence of a large background of other chemical species, 2) finding ways to incorporate many different selective groups into a single polymer, 3) fabricating polymer films, strips, sheets, and coatings that can be applied to other materials, such as fiber optics and surfaces, 4) developing interfaces between the polymers and substrates that can be used to produce prototype arrays of many sensor elements for rapid multi-contaminant detection and quantitation, and 5) developing multiplexed data collection techniques to rapidly process the data obtained from many polymer sensors into a chemical profile of a waste stream or waste site in real time. Each project is designed to carry out an important aspect of sensor development that will be integrated into an overall effort to produce novel sensors for use in the rapid assessment of environmental remediation strategies.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§ ID-WM-107	C-45	Long Term Treatment/Storage/Disposal Operations
§ RL-WM03	C-193	Solid Waste Storage and Disposal
§ RL-WM04	C-197	Solid Waste Treatment
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW02	C-285	Transuranic Waste Project
§+ SR-SW03	C-287	Mixed Low Level Waste Project
AL024	C-3	Grand Junction Office (GJO) All Other Projects
AL007	C-7	Environmental Restoration
+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
NV212	C-49	Underground Test Area (UGTA)
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
OR-43204	C-77	ORNL Bethel Valley Deactivation and Decommissioning
+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ OR-45301	C-103	Paducah Remedial Action
+ OR-46301	C-107	Portsmouth Remedial Action
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
RL-ER08	C-147	Groundwater Management
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW04	C-169	Retrieval Project
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project
+ SR-HL01	C-249	H-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure

Environmental Management Science Program Research in Illinois

Argonne National Laboratory

55294-IL - Superconducting Open-Gradient Magnetic Separation for the Pretreatment of Radioactive or Mixed Waste Vitrification Feeds

Year of Award: 1996 **Amount of Award:** $1,500,000
Problem Area: High Level Waste
Science Category/SubCategory: Engineering Science / Diagnostics
Principal Investigator: Richard D. Doctor, 630-252-5913, richard_doctor@qmgate.anl.gov
Major Collaborator(s): C. A. Cicero-Herman at Savannah River Technology Center
J. A. Ritter at the University of South Carolina
S. Landsberger at the University of Texas at Austin
For More Information: http://www.doe.gov/em52/55294.html

Description Provided by Investigator:

Scientists need to gain a better understanding of the magnetic separation processes that can be used to separate deleterious constituents (crystalline, amorphous, and colloidal) in vitrification feed streams for borosilicate glass production without adding chemicals or generating secondary waste streams. This field work research describes how Argonne research staff and their partners will combine fundamental science with basic engineering to determine how magnetic separation can best be used for pretreatment of radioactive and mixed-waste vitrification feed streams. The results of this work will be used to reduce the volume and cost of high-level waste glass produced during U.S. Department of Energy (DOE) remediation activities. By elucidating the magnetic properties of constituents and their interactions with the chemical and physical environment, researchers will be better able to develop reliable models and efficient magnetic separation processes. Our proposed multidisciplinary technical approach involves using physical and chemical techniques to identify the magnetic constituents and radionuclides in the waste streams. The project will include the systematic study of magnetic interactions of waste constituents under controlled physical and chemical conditions (e.g., hydration, oxidation, temperature) to identify the mechanisms that control the magnetic properties. We will also study the partitioning of the radionuclides to determine their sorption mechanisms. The identification of fundamental magnetic properties within the microscopic chemical environment will be combined with development of hydrodynamic and electrodynamic models to understand the microscopic parameters for optimal magnetic separation. This project will lead to the effective use of superconducting open-gradient magnetic separation as a pretreatment technique for radioactive or mixed-waste vitrification feeds from DOE sites.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

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Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§ ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ RL-TW08	C-185	Process Waste Privatization Infrastructure
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
§ SR-HL05	C-265	Vitrification
AL024	C-3	Grand Junction Office (GJO) All Other Projects
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-48101	C-99	Offsite Remedial Action
+ OR-45301	C-103	Paducah Remedial Action
RL-ER08	C-147	Groundwater Management
RF014	C-213	Industrial Zone Closure Project
+ SR-ER06	C-227	Upper Three Runs Project
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in Illinois

Argonne National Laboratory

55367-IL - Investigation of Microscopic Radiation Damage in Waste Forms Using ODNMR and AEM Techniques

Year of Award: 1996 **Amount of Award:** $698,000
Problem Area: High Level Waste
Science Category/SubCategory: Materials Science / Radiation Effects On Storage Materials
Principal Investigator: Dr. Guokui Liu, 630-252-4630, gliu@anlchm.chm.anl.gov
For More Information: http://www.doe.gov/em52/55367.html

Description Provided by Investigator:

The proposed project addresses DOE nuclear waste problems that are currently intractable without achieving a fundamental understanding of radiation effects on high level waste (HLW) forms. This project will investigate the microscopic effects of radiation damage in crystalline and glass forms. Information about the nature of electronic interaction and the chemical bonding properties of radionuclides in damaged phases will be provided. Connections between the consequences of alpha and beta-decay processes and radionuclide release and chemical decomposition in waste forms will be established. Detailed studies will focus on the microscopic effects of alpha-decay of the transuranic isotopes ^{238,239}Pu, ^{241,243}Am, and ^{243,244}Cm and the beta- and alpha-decay of ^{249}Bk(^{249}Cf) doped into crystalline materials 10 to 30 years ago and currently prepared borosilicate glasses. Electronic and chemical binding properties and local structural changes of parent radionuclide species and their decay daughters in the radiation damaged regions of the waste forms will be probed using, nonlinear laser spectroscopic techniques, such as optically detected nuclear magnetic resonance (ODNMR), in concert with analytical electron microscopy (AEM) imaging and analysis and X-ray diffraction methods. Experimental information obtained using various techniques for the same materials will be compared and systematic measurements will be made after the samples undergo a series of annealing tests. Theoretical models based on electronic and nuclear interactions of the actinides and their surrounding ligands will be developed to interpret the experimental results and correlate the microscopic effects of radiation damage to the macroscopic mechanical and chemical properties of the HLW materials.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

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Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§ ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ RL-TW08	C-185	Process Waste Privatization Infrastructure
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§ SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Illinois

Argonne National Laboratory

55374-IL - Use of Sonication for In-Well Softening of Semivolatile Organic Compounds

Year of Award: 1996 **Amount of Award:** $1,470,000
Problem Area: Remedial Action
Science Category/SubCategory: Engineering Science / Bubble Mechanics and Sonification
Principal Investigator: Dr. Robert W. Peters, 630-252-7773, robert_peters@qmgate.anl.gov
Major Collaborator(s): John Manning at Argonne National Laboratory
Michael Hoffmann at the California Institute of Technology
Steven Gorelick at Stanford University
For More Information: http://www.doe.gov/em52/55374.html

Description Provided by Investigator:

The specific objectives of the proposed work are to investigate the in-situ degradation of semivolatile organic compounds (SVOCs) and to:

- Determine the system performance of the combination of in-well sonication, vapor stripping, and biodegradation to destroy VOCs and change SVOCs into VOCs;
- Determine how the combined in-well vapor stripping, sonication, and in-situ biodegradation remedial system functions together at the laboratory scale to remove SVOCs and VOCs;
- Determine the chemical reaction mechanisms for destroying VOCs and changing the SVOCs to VOCs, and improve the overall system performance;
- Quantify the roles of the individual treatment components (sonication, in-well vapor stripping, and biodegradation) on the overall effectiveness of the remediation, and acceleration. It deals with novel bioremediation reactions, alternative electron acceptor conditions, and modeling the remedial system;
- Determines, after water is treated in the well with sonication and VOCs are partially removed through in-well vapor stripping, the role of volatilization and microbial activity on water containing VOCs that is forced to infiltrate through the unsaturated zone;
- Determine the effect of sonication/megasonics on well corrosion, and
- Identify the appropriate system design for scale-up of the remedial system for demonstration in the field and deployment.

This project has as its goal the partial degredation (i.e., "softening") of the more recalcitrant organic compounds (e.g., SVOCs and nonvolatile organic compounds) in order to convert them into compounds that are more amenable to both vapor stripping and biological treatment. The SVOCs are not effectively removed from solution by using air sparging techniques. Conversion of SVOCs to VOCs could allow effective removal of the organics with vacuum extraction techniques or in-situ biotreatment This project investigates the combined treatment using in-well sonication, in-well vapor stripping, and biodegradation. The proposed work will examine the use of sound-wave energies (e.g., ultrasonics and megasonics) to transform the SVOCs to VOCs. Performing the partial degredation (i.e., "softening") in-well would permit the treated organics to be reinjected and percolated through the subsurface, thereby enhancing biodegradation rates by generating organics that are more easily biodegraded. Successful implementation of such an approach would considerably reduce both the time and cost of in-situ biotreatment. Pretreating groundwaters by means of sonication techniques would form VOCs that could be removed effectively by either bioremediation technologies or a dual vapor extraction technique (being developed by Stanford University under the VOC-Arid Program, now part of the Plumes Focus Area). Sonication could also be coupled with technologies, such as surfactant flooding, aimed at mobilizing dense non-aqueous-phase liquids (DNAPLs) in the subsurface.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

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Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ OR-46301	C-107	Portsmouth Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Illinois

Argonne National Laboratory

55380-IL - In-Situ Spectro-Electrochemical Studies of Radionuclide Contaminated Surface Films on Metals and the Mechanism of their Formation and Dissolution

Year of Award: 1996 **Amount of Award:** $1,005,000
Problem Area: Decontamination and Decommissioning
Science Category/SubCategory: Materials Science / Surface Chemistry
Principal Investigator: Dr. Carlos A. Melendres, 630-252-4346, MELENDRES@AXP.CMT.ANL.GOV
Major Collaborator(s): S. M. Mini at Northern Illinois University
For More Information: http://www.doe.gov/em52/55380.html

Description Provided by Investigator:

The aim of this research is to gain a fundamental understanding of the structure, composition, and mechanism of formation of radionuclide-containing surface films on metals that are relevant to the problem of decontamination of piping systems and waste storage tanks at DOE nuclear facilities. This project seeks to expand our knowledge, while obtaining useful practical information, through the conduct of a systematic research activity that utilizes the unique facilities at Argonne National Laboratory, e.g., the Advanced Photon Source (APS) for x-ray absorption spectroscopy (XAS), as well as specialized laboratory facilities and instrumentation for carrying out experiments with radioactive materials. Formal collaboration with a university assures that a strong basic approach is taken in the analyses and methodologies used to achieve the desired goals.

Electrochemical studies will be carried out on the corrosion and passivation behavior of iron, nickel, chromium, and stainless steel over a wide pH range and as a function of temperature from 25 to 95°C. The energetics and dynamics of film formation and dissolution and the effect of incorporation of heavy metal ions and radioactive elements will be investigated. Synchrotron x-ray absorption and vibrational (infrared and Raman) spectroscopic techniques will be used to define "in-situ" the structure and composition of the various oxide phases that are formed as a function of temperature.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Decontamination and Decommissioning problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Decontamination and Decommissioning".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
§ OR-43204	C-77	ORNL Bethel Valley Deactivation and Decommissioning
§ OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
§+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
§+ RL-ER06	C-141	Decontamination and Decommissioning
§+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
§ RL-TP10	C-163	Accelerated Deactivation
RL-ER08	C-147	Groundwater Management
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II

Environmental Management Science Program Research in Illinois

Argonne National Laboratory

55382-IL - Determination of Transmutation Effects in Crystalline Waste Forms

Year of Award: 1996 **Amount of Award:** $912,985
Problem Area: Nuclear Materials
Science Category/SubCategory: Materials Science / Radiation Effects On Storage Materials
Principal Investigator: Dr. Denis M. Strachan, 630-252-4479, strachand@cmt.anl.gov
Major Collaborator(s): Dr. Nancy J. Hess at Pacific Northwest National Laboratory
For More Information: http://www.doe.gov/em52/55382.html

Description Provided by Investigator:

The objective of this study is to characterize the effects of transmutation in a candidate waste form for ^{137}Cs by investigating samples of a cesium aluminosilicate mineral, pollucite, that have undergone "natural" decay of the Cs under ambient temperature while isolated from interfering chemical effects. There currently is no information on β-decay transmutation effects in waste forms in which transmutation has occurred over the natural decay time of the decaying isotope. This causes large uncertainty as to the effect of the transmutation on the physical and chemical properties of the waste form. As a result, uncertainties arise about the viability of the waste form as a long-term storage media for nuclear waste. Information on the effects of transmutation from α-decay will give support to the selection of alternate waste forms for separated ^{137}Cs and give information on the long-term behavior of candidate waste forms.

The approach that will be taken is to nondestructively examine small stainless steel capsules containing pure pollucite. The contents of these capsules will be examined with XANES, XAFS, and small angle anomalous x-rays. The synchrotron facilities at Stanford and ANL will be utilized. The scientific team is comprised of members from PNNL, ANL, and LANL.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Nuclear Materials problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Nuclear Materials".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ RL-TP07	C-161	Plutonium Finishing Plant (PFP) Vault Management
ID-HLW-101	C-29	High-Level Waste Pretreatment
ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
+ RL-TW04	C-169	Retrieval Project
+ RL-TW05	C-173	Process Waste Support
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
+ RL-TW08	C-185	Process Waste Privatization Infrastructure
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
+ SR-HL01	C-249	H-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Illinois

Argonne National Laboratory

55388-IL - Stable Isotopic Investigations of in situ Bioremediation of Chlorinated Organic Solvents

Year of Award: 1996 **Amount of Award:** $825,000
Problem Area: Remedial Action
Science Category/SubCategory: Biogeochemistry / Biogeochemistry
Principal Investigator: Dr. Neil C. Sturchio, 630-252-3986, sturchio@anl.gov
For More Information: http://www.doe.gov/em52/55388.html

Description Provided by Investigator:

We propose to develop innovative methods for investigating the mechanism and extent of *in situ* bioremediation of chlorinated organic solvents. These methods will use precise isotopic ratio measurements of chlorine and carbon in reactant and product species in laboratory experiments and in materials from field demonstration sites. Specific tasks will include (1) optimization of the sampling and analytical methods for determining compound-specific chlorine and carbon isotope ratios in the appropriate chemical systems; (2) definition of the chlorine and carbon isotopic fractionation factors during biological degradation of chlorinated solvents in laboratory experiments; and (3) use of chlorine and carbon isotope ratios to investigate biodegradation of chlorinated solvents at field demonstration sites where contrasting *in situ* bioremediation schemes are being employed. This work is relevant to EMSP goals because it will provide a new and cost-effective means of evaluating and monitoring the effectiveness of *in situ* bioremediation schemes for chlorinated solvents in soils, vadose horizons, and groundwater plumes.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§ RL-ER08	C-147	Groundwater Management
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Illinois

Argonne National Laboratory

60283-IL - Waste Volume Reduction Using Surface Characterization and Decontamination by Laser Ablation

Year of Award: 1997 **Amount of Award:** $790,000
Problem Area: Decontamination and Decommissioning
Science Category/SubCategory: Separations Chemistry / Ligand Design and Ion-exchange
Principal Investigator: Dr. Michael J. Pellin, 630-252-5217, pellin@anl.gov
For More Information: http://www.doe.gov/em52/60283.html

Description Provided by Investigator:

The waste stream generated in the decontamination and decommissioning (D&D) of nuclear facilities includes a significant volume of material that is contaminated only in the surface or near-surface region. The U.S. Department of Energy will require disposal of as mush as 10^9 ft^2 (and 10^7 ft^3) of contaminated concrete in the next 20 years. In order to design efficient, cost-effective D&D of these facilities, it is critical to understand the depth-dependent concentration and chemistry of radionuclide-contaminated surfaces. Complete removal and capture of the contaminated surface would greatly reduce the volume of waste material generated in D&D efforts.

Here, unique quantitative surface analytical capabilities are used to measure the depth-dependent radionuclide concentrations of test surfaces that represent the full range of materials and exposures found in nuclear facilities. These studies represent the first detailed surface studies of the sorption of radionuclides in complex material such as concrete. This information, along with the chemical state of the contaminant, will provide a useful resource in the design and application of surface removal instruments. Because laser ablation is part of the analysis method, information derived here will allow analysis of contaminants on line via mass spectrometry when laser removal systems are used for D&D.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Decontamination and Decommissioning problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Decontamination and Decommissioning".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
§ OR-43204	C-77	ORNL Bethel Valley Deactivation and Decommissioning
§ OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
§+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
§+ RL-ER06	C-141	Decontamination and Decommissioning
§+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RF014	C-213	Industrial Zone Closure Project

Environmental Management Science Program Research in Illinois

Argonne National Laboratory

60313-IL - Radiation Effects on Transport and Bubble Formation in Silicate Glasses

Year of Award: 1997 **Amount of Award:** $750,000
Problem Area: High Level Waste
Science Category/SubCategory: Separations Chemistry / Catalyst Chemistry and Waste Treatment
Principal Investigator: Dr. Alexander D. Trifunac, 630-252-4993, trifunac@anlchm.chm.anl.gov
For More Information: http://www.doe.gov/em52/60313.html

Description Provided by Investigator:

The objective of the research is to discover the molecular details of chemistry induced by β-, γ-, and neutron-irradiation of silicate glasses. The ionization and ballistic effects of radiation will be studied from the viewpoint of defect formation and transport properties. Dose and dose-rate effects will be investigated under temperature conditions expected to occur in the geological repository. Special emphasis will be given to molecular processes crucial for understanding the aggregation of defects and formation of oxygen bubbles. Radiation-induced oxidation/reduction of metal ions involved in glass leaching will be studied. The fundamental knowledge gained will help to provide the necessary scientific basis for extrapolating the long-term behavior of stored radioactive waste glass forms. Our group possesses a wide range of special tools to detect and characterize species important for (i.e., pulse radiolysis, laser photolysis, time-resolved optical spectroscopy, and Raman scattering) will be complimented by our unique time-resolved magnetic resonance facilities. The research will be coordinated with, and performed in collaboration with, the ongoing EMSP projects at Pacific Northwest National Laboratory (W.J. Weber) and the Naval Research Laboratory (D.L. Griscom).

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§ ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§+ RL-TW08	C-185	Process Waste Privatization Infrastructure
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§ SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Illinois

Illinois Institute of Technology

60143-IL - Foaming in Radioactive Waste Treatment and Immobilization Processes

Year of Award: 1997 **Amount of Award:** $360,360
Problem Area: High Level Waste
Science Category/SubCategory: Engineering Science / Bubble Mechanics and Sonification
Principal Investigator: Dr. Darsh T. Wasan, 312-567-3001, wasan@iit.edu
For More Information: http://www.doe.gov/em52/60143.html

Description Provided by Investigator:

The physical mechanisms of the formation of foam in radioactive waste treatment and waste immobilization processes are poorly understood. The objective of this research is to develop a basic understanding of the mechanisms that produce foaming, to identify the key parameters which aggravate foaming, and to identify effective ways to eliminate or mitigate foaming. A unique feature of this study lies in the use of its newly developed instrumental techniques including differential microinterferometry, film rheometry, and capillary force balance. The specific tasks to be undertaken are: (1) to establish the effects of colloidal particles, inorganic and organic components on foam formation and stability. The effects of particles' hydrophobicity and hydrophilicity, and chemical flocculents and defoamers on foaming will be elucidated; (2) to examine particle-particle and particle-foam lamella interactions using the novel capillary force balance apparatus; (3) to determine the dynamic film tension and film elasticity using the newly designed film rheometer; and (4) to monitor the vertical film drainage rate using the reflected light interferometry. Systems to be investigated will include simulated waste materials as well as pure compounds. The results of this study will aid in significantly enhancing our understanding of foam technology in three phase gas/liquid/solid systems and thereby facilitating implementation of environmental technologies for radioactive waste treatment and waste immobilization processes.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§ SR-HL05	C-265	Vitrification
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in Illinois

University of Illinois at Chicago

60247-IL - Miniature Nuclear Magnetic Resonance Spectrometer for In-Situ and In-Process Analysis and Monitoring

Year of Award: 1997 **Amount of Award:** $482,000
Problem Area: Nuclear Materials
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Sensors and Techniques
Principal Investigator: Dr. Gennady Friedman, 312-413-0827, gary@eecs.uic.edu
For More Information: http://www.doe.gov/em52/60247.html

Description Provided by Investigator:

The objective of this research project is to develop a new analytical instrument based on the principle of nuclear magnetic resonance (NMR) for in-situ, in-field and in-process characterization and monitoring of various substances and chemical processes. The new instrument will be a highly miniaturized version an NMR spectrometer and its development will involve application of the most recent advances in the fields of micromachining and microfabrication, permanent magnet materials and design, and microelectronics and signal processing. The proposed miniature NMR spectrometer will be a hand-held unit weighing around 5-6 pounds and intended to perform measurements on liquid samples of micro- to nano-liter volumes. The resolution of the instrument is projected to be better than 0.1 ppm (part per million) with sensitivities approaching 10 to 100 ppm (1 millimolar to 10 millimolar) for proton containing molecules. While initial developments will focus on applications of proton NMR, further developments will be aimed at other nuclei, such as 19F, 31P and 13C. Applications of the miniature NMR system will include down hole monitoring of ground water pollutants and flow, real-time in-process monitoring of waste remediation activities, spatial composition analysis in chemical and waste storage tanks, in-field characterization of waste materials and many others.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Nuclear Materials problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Nuclear Materials".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
AL007	C-7	Environmental Restoration
+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
ID-HLW-101	C-29	High-Level Waste Pretreatment
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
ID-WM-107	C-45	Long Term Treatment/Storage/Disposal Operations
NV214	C-53	Industrial Sites
+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ OR-45301	C-103	Paducah Remedial Action
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW04	C-169	Retrieval Project
+ RL-TW05	C-173	Process Waste Support
+ RL-TW07	C-181	Process Waste Privatization Phase II
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
RL-WM03	C-193	Solid Waste Storage and Disposal
RL-WM04	C-197	Solid Waste Treatment
RF014	C-213	Industrial Zone Closure Project
+ SR-HL01	C-249	H-Tank Farm
+ SR-HL02	C-253	F-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
SR-HL05	C-265	Vitrification
+ SR-SW01	C-281	Consolidated Incinerator Facility
+ SR-SW02	C-285	Transuranic Waste Project
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in Illinois

University of Illinois at Urbana-Champaign

55211-IL - Cavitational Hydrothermal Oxidation: A New Remediation Process

Year of Award: 1996 **Amount of Award:** $478,027
Problem Area: Mixed Waste
Science Category/SubCategory: Engineering Science / Bubble Mechanics and Sonification
Principal Investigator: Dr. Kenneth S. Suslick, 217-333-2794, ksuslick@uiuc.edu
For More Information: http://www.doe.gov/em52/55211.html

Description Provided by Investigator:

This research will explore the emerging science of sonochemistry and its technological applications for organic waste remediation, particularly for water and soil purification. Ultrasound can induce unusual high-energy chemistry through the process of acoustic cavitation: the formation, growth, and *implosive collapse* of bubbles in a liquid. Cavitation can occur both in clouds of collapsing bubbles (multi-bubble cavitation, MBC) or with high symmetry for isolated bubble (single-bubble cavitation, SBC). Multi-bubble cavitational collapse produces localized, transient hot spots with *intense* local heating (~5000K), high pressures (~2000 atm), and short lifetimes (sub-microsecond) in an otherwise cold liquid. From hydrodynamic modeling of this cavitational collapse, we can estimate that both the heating and cooling rates are in excess of 10^{10} K/sec, which is faster than splat-cooling of molten metals onto liquid He cooled surfaces! Acoustic cavitation is a unique means of creating high energy chemistry, easily and inexpensively. Aqueous sonochemistry produces, on a *microscopic* scale, supercritical water conditions with a vengeance! The applications of cavitation to remediation of toxic organics, however, has only begun to be explored in a convincing fashion.

In this regime of temperature and pressure, the sonochemistry of water is an extreme limiting case of supercritical phenomena and is closely related to hydrothermal oxidation (HTO). For example, the ultrasonic irradiation of water produces a variety of extraordinarily reactive species (including OH*, H*, and HO_2) capable of decomposing essentially all organic compounds. Furthermore, the temperatures reached in the cavitation hot spots are sufficient to pyrolyze all volatile organic compounds.

Our overall goal in this research is to develop our understanding of the reactions of organic compounds in the presence of high intensity ultrasound. Our specific objectives in this proposed work fall into four areas: 1) investigation of the local conditions formed during cavitation in water; 2) mechanistic examination of the effects of cavitation on polycyclic aromatic hydrocarbons, nitroaromatics, and halocarbons; 3) determination of degradation yields as a function of experimental configurations of aromatics and halocarbons as toxic impurities in water, and 4) design and testing of large scale flow processing systems useful for remediation of contaminated water. In all cases, we will continue our special emphasis on the mechanistic origins of sonochemistry, in relationship to its applications to environmental challenges. Information gained should lead to effective protocols and equipment designs for large scale treatment of contaminated water and soil slurries

The Pimentel Report ("Opportunities in Chemistry", National Research Council) in their *first* recommendation noted five research frontiers which should receive priority: one of these is "Chemical Behavior Under Extreme Conditions". The committee stated our thesis perfectly:*"We propose an initiative to explore chemical reactions under conditions far removed from normal ambient conditions. Chemical behaviors under extreme pressures, extreme temperatures, ... provide critical tests of our basic understandings of chemical reactions and new routes toward discovery of new materials and new devices"* (p. 12). Chemistry, after all, is the interaction of energy and matter, and the energy source often determines chemical reactivity. One way of representing these interactions is to visualize a three-dimensional space with axes of pressure vs. energy vs. time of interaction. Sonochemistry provides a unique access to regions of this reactivity-space and represents a distinct class of interaction of energy and matter. Ultrasound induces this unusual high-energy chemistry through the process of acoustic cavitation: the formation, growth, and *implosive collapse* of bubbles in a liquid. Acoustic cavitation is the underlying phenomenon which is responsible for sonochemistry and sonoiuminescence.

In spite of early work in the area of sonochemistry, interest within the chemical community remained exceedingly modest until the 1980's. With the advent of inexpensive and reliable sources of ultrasound, however, sonochemistry has undergone a dramatic renaissance. As our understanding of the nature of the chemical effects of ultrasound has grown, so too has the impact of sonochemistry on the chemical community. We have discovered a variety of chemical consequences of these phenomena, including dramatic improvements in both catalytic and stoichiomrtric reactions of organometallics, metal surfaces, and semiconductor powders. We have developed unique sonochemical syntheses of novel amorphous and nanophase materials unavailable by other techniques. And, we have found important biomedical applications involving sonochemical production of proteinaceous microspheres. Thus the scientific impact of sonochemistry has promise in a wide range of the physical sciences.

Sonochemistry also has substantial *strategic research significance* to our industrial economy. Ultrasound has already major industrial applications, and the U.S. completely dominates the world market in the production of ultrasonic equipment. Commercial ultrasound equipment for large scale liquid processing is available off-the-shelf at quite modest costs. It is extremely important in solids processing, including cutting, welding, cleaning and precipitation. Ultrasonic cleaning, for example, now dominates both general purpose industrial and microelectronics applications, due to increasing restrictions on the use of halocarbon and other organic solvents. Ultrasound is an already established technology for industrial emulsification, solvent degassing, solid dispersion, cell disruption, and sol formation (e.g., fume scrubbers).

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW03	C-287	Mixed Low Level Waste Project
AL024	C-3	Grand Junction Office (GJO) All Other Projects
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ OR-48101	C-99	Offsite Remedial Action
+ OR-45301	C-103	Paducah Remedial Action
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
RL-ER08	C-147	Groundwater Management
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Indiana

Purdue University

54834-IN - An Investigation of Homogeneous and Heterogeneous Sonochemistry for Destruction of Hazardous Waste

Year of Award: 1996 **Amount of Award:** $290,000
Problem Area: Remedial Action
Science Category/SubCategory: Inorganic Chemistry / Multiphase/Gaseous Chemistry
Principal Investigator: Dr. Inez Hua, 317-494-2409, hua@ecn.purdue.edu
For More Information: http://www.doe.gov/em52/54834.html

Description Provided by Investigator:

During the last 20 years, various legislative acts have mandated the reduction and elimination of water and land pollution. In order to fulfill these mandates, effective control and remediation methods must be developed and implemented. The drawbacks of current hazardous waste control methods motivate the development of new technology, and the need for new technology is further driven by the large number of polluted sites across the country. This research explores the application and optimization of ultrasonic waves as a novel method by which aqueous contaminants are degraded.

The primary objective of the investigation is to acquire a deeper fundamental knowledge of acoustic cavitation and cavitation chemistry, and in doing so, to ascertain how ultrasonic irradiation can be more effectively applied to environmental problems. Special consideration is given to the types of problems and hazardous chemical substrates found specifically at Department of Energy (DOE) sites.

The experimental work is divided into five broad tasks, to be completed over a period of three years. The first task is to explore the significance of physical variables during sonolysis, such as ultrasonic frequency. The second aim is an understanding of sonochemical degradation kinetics and by-products, complemented by information from the detection of reactive intermediates with electron paramagnetic resonance. The sonolytic decomposition studies will focus on polychlorinated biphenyls (PCBs). Investigation of activated carbon regeneration during ultrasonic irradiation extends sonochemical applications in homogeneous systems to heterogeneous systems of environmental interest. Lastly, the physics and hydrodynamics of cavitation bubbles and bubble clouds will be correlated with sonochemical effects by performing high-speed photographic studies of acoustically cavitating aqueous solutions. The most important benefit will be fundamental information which will allow a more optimal application of ultrasonic irradiation to environmental problems.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ NV214	C-53	Industrial Sites
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER02	C-129	200 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ RF014	C-213	Industrial Zone Closure Project
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
SR-HL05	C-265	Vitrification
+ SR-SW01	C-281	Consolidated Incinerator Facility
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in Indiana

University of Notre Dame

54576-IN - On the Inclusion of the Interfacial Area Between Phases in the Physical and Mathematical Description of Subsurface Multiphase Flow

Year of Award: 1996 **Amount of Award:** $845,252
Problem Area: Remedial Action
Science Category/SubCategory: Hydrogeology / Instrumentation and Modelling
Principal Investigator: Dr. William G. Gray, 219-631-5942, wggray@gauss.ce.nd.edu
Major Collaborator(s): Dr. Andrew 'Andy' Tompson at Lawrence Livermore National Laboratory
Dr. Wendy E. Soll at Los Alamos National Laboratory
For More Information: http://www.doe.gov/em52/54576.html

Description Provided by Investigator:

A distinguishing feature of multi-phase subsurface flow in comparison to single phase flow is the existence of fluid-fluid interfaces. These interfaces define phase boundaries at the pore scale and influence overall system behavior in many important ways. For example, fluid-fluid interfaces support non-zero stresses, allowing for different phase pressures across each interface. In problems of inter-phase mass transfer, such as evaporation in air-water systems or dissolution in hydrocarbon-water systems, all mass is exchanged via the interfaces. While interfaces are central to multi-phase flow physics and associated contaminant transport, their treatment in traditional porous-media theories has been given little attention. Recent theoretical work provides a general framework within which interfacial area is incorporated explicitly into volume-averaged equations for conservation of mass, momentum, and energy. This leads to an expanded set of continuum-scale equations that carry the overhead burden of the associated set of expanded constitutive relationships. To make these equations a scientifically useful tool for the study of the soil environment, parameterization of the constitutive forms must occur. This parameterization requires that the equations be studied in light of the actual behavior of porous media systems. To perform the early stages of this work effectively, the porous media must be controlled, well-understood systems that lend themselves to careful scientific analysis. The present research will contribute to the improved understanding and precise physical description of multiphase subsurface flow by combining theoretical derivation of equations, lattice Boltzmann modeling of hydrodynamics to identify characteristics and parameters (see also research by Dr. Wendy E. Soll at LANL), and solution of the field-scale equations using a discrete numerical method to assess the advantages and disadvantages of the complete theory (see also research by Dr. Andrew Tompson at LLNL). This approach includes both fundamental scientific inquiry and a path for inclusion of the scientific results obtained in a technical tool that will improve assessment capabilities for multiphase flow situations that have arisen due to spills of organic materials in the natural environment.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ NV212	C-49	Underground Test Area (UGTA)

Environmental Management Science Program Research in Indiana

University of Notre Dame

54942-IN - Spectroscopy, Modeling and Computation of Metal Chelate Solubility in Supercritical CO2

Year of Award: 1996 **Amount of Award:** $300,000
Problem Area: Mixed Waste
Science Category/SubCategory: Separations Chemistry / Ligand Design and Ion-exchange
Principal Investigator: Dr. Joan F. Brennecke, 219-631-5847, JFB@VYASA.HELIOS.ND.EDU
Major Collaborator(s): Dr. Mark A. Stadtherr at the University of Notre Dame
John E. Chateauneuf at Western Michigan University
For More Information: http://www.doe.gov/em52/54942.html

Description Provided by Investigator:

Objectives

The objectives of this project are to gain a fundamental understanding of the solubility and stability of metal chelates in supercritical CO_2. Extraction with CO_2 is a excellent way to remove organic compounds from soils, sludges and aqueous solutions and recent research has demonstrated that together with chelating agents it is a viable way to remove metals, as well. The fundamental knowledge gained will be vital to computing phase behavior, and modeling and designing processes using CO_2 to separate organics and metal compounds from DOE mixed wastes. We are pursuing a comprehensive program to measure local solvation of metal chelates and to determine metal chelate stability in supercritical fluid mixtures using UV-vis and FTIR spectroscopy. These spectroscopic studies will provide information on the solution microstructure, which will be used in concert with published solubility data to evaluate and develop thermodynamic models of the solubility behavior. Finally, we are implementing a more reliable computational technique, based on interval mathematics, to compute the phase equilibria using the thermodynamic models. This will be important in the design of processes using CO_2 to extract components from mixed wastes and in determining the optimum operating conditions.

Introduction and Significance

The overall objectives of this project are to gain a fundamental understanding of the solubility and stability of metal chelates in supercritical CO_2 and to use that understanding to model and compute phase behavior. This is necessary to design processes using CO_2 to separate organics and metal compounds from DOE mixed wastes. Many mixed wastes that are stored and produced at various DOE sites are not amenable to direct treatment. They may contain oils, greases, hazardous organic and inorganic compounds, metals, radioactive materials, heavy metals in the form of solids, liquids and sludges and decontamination wastes (cloth, plastic, paper). The Hanford site alone hosts 177 single- and double-shell tanks containing liquid, solid and sludge mixed wastes and has up to 1500 m^3 of solid wastes for which there is no currently available or acceptable treatment due to the combination of waste contaminants present. Separation of the wastes into components makes them much easier to treat by technologies such as vitrification, incineration, and low temperature oxidation.

Background and Proposed Studies

Extraction with supercritical CO_2 is an attractive possibility for the separation of DOE mixed wastes. Carbon dioxide is nontoxic and nonflammable and extraction with CO_2 has been successful for the decaffeination of coffee and tea, recovery of hops, edible oils and other natural products, the regeneration of activated carbon, the separation of organic solutions, and the fractionation of polymers. Supercritical CO_2 has also been used for the selective extraction of compounds from soils and other solid matrices. Based on preliminary investigations at Rocky Flats and the University of Colorado, extraction with CO_2 has been proposed as a way to separate organics from DOE low-level mixed wastes at Hanford and Rocky Flats. However, an important issue is the fate of the metal compounds. The seminal work of several research groups over the last decade has shown not only that some metal chelates are sufficiently solubility in CO_2 or CO_2/cosolvent mixtures, but that metals can be successfully extracted from aqueous solutions and solid matrices with CO_2. Since many metal chelates have significantly lower solubilities in CO_2 than most organics, one can envision a process in which both organics and metal chelates are extracted at a relatively high pressure (e.g., 3000-5000 psi). The metal compounds could be selectively separated by partial depressurization. The organics would be deposited upon further expansion of the CO_2. Alternatively, one could devise a two-step extraction in which the organics were removed first and then the metals were removed by adding the chelating agent to the CO_2 solvent stream.

In this project we are focusing on three areas of fundamental interest that are important in the development of this technology and that have not yet been adequately addressed. First, we plan to use UV-vis and FTIR spectroscopy to measure preferential solvation of metal chelates in SC mixtures and to study the stability of the various metal chelates in SC CO_2 and SC CO_2 mixtures as a function of temperature, pressure and cosolvent. Second, we plan to use this information in concert with published solubility data to develop more successful models of the metal chelate solubilities in the SCF phase. Third, and as a complement to the modeling efforts, we plan to implement a completely reliable computational method using interval mathematics to calculate the solubilities using the thermodynamic models that are developed. Our work using spectroscopy to characterize these compounds and their stability and to model and compute the solubilities is a vital complement to previous work, and is necessary in developing a fundamental basis for technology using CO_2 to separate metals and organics.

This project is a collaborative effort between Dr. Joan F. Brennecke and Dr. Mark A. Stadtherr at the University of Notre Dame and Dr. John E. Chateauneuf in the Department of Chemistry at Western Michigan University (phone: 616-387-2879; fax: 616-387-2909; E-mail: chateauneuf@wmich.edu).

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW03	C-287	Mixed Low Level Waste Project
NV214	C-53	Industrial Sites
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Indiana

University of Notre Dame

59934-IN - Hazardous Gas Production by Alpha Particles in Solid Organic Transuranic Waste Matrices

Year of Award: 1997 **Amount of Award:** $400,362
Problem Area: Mixed Waste
Science Category/SubCategory: Inorganic Chemistry / Multiphase/Gaseous Chemistry
Principal Investigator: Dr. Jay A. LaVerne, 219-631-5563, laverne.1@nd.edu
For More Information: http://www.doe.gov/em52/59934.html

Description Provided by Investigator:

This project proposes to use fundamental radiation chemical techniques to elucidate the basic processes occurring in the heavy-ion radiolysis of solid hydrocarbon matrices such as polymers and organic resins that are associated with many of the transuranic waste deposits or the transportation of these radionuclides. The environmental management of mixed waste containing transuranic radionuclides is difficult because these nuclides are alpha particle emitters and the energy deposited by the alpha particles causes chemical transformations in the matrices accompanying the waste. Most radiolysis programs focus on conventional radiation such as gamma rays, but the chemical changes induced by alpha particles and other heavy ions are typically very different and product yields can vary by more than an order of magnitude. The objective of this research is to measure the production of gases, especially molecular hydrogen, produced in the proton, helium ion, and carbon ion radiolysis of selected solid organic matrices in order to obtain fundamental mechanistic information on the radiolytic decomposition of these materials. This knowledge can also be used to directly give reasonable estimates of explosive or flammability hazards in the storage or transport of transuranic wastes. The research proposed here utilizes the unique facilities of the Notre Dame Radiation Laboratory to provide both basic knowledge of and practical information on systems important to the Environmental Management Science Program of the Department of Energy that is not likely to otherwise be obtained.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-107	C-45	Long Term Treatment/Storage/Disposal Operations
§ RL-WM03	C-193	Solid Waste Storage and Disposal
§ RL-WM04	C-197	Solid Waste Treatment
§+ SR-SW02	C-285	Transuranic Waste Project
§+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in Indiana

University of Notre Dame

59960-IN - Direct Investigations of the Immobilization of Radionuclides in the Alteration Phases of Spent Nuclear Fuel

Year of Award: 1997 **Amount of Award:** $782,487
Problem Area: Spent Nuclear Fuel
Science Category/SubCategory: Geochemistry / Solid/Solution Geochemistry
Principal Investigator: Dr. Peter C. Burns, 219-631-5380, Peter.Burns.50@nd.edu
Major Collaborator(s): Dr. Robert J. Finch at Argonne National Laboratory
David J. Wronkiewicz at the University of Missouri-Rolla
For More Information: http://www.doe.gov/em52/59960.html

Description Provided by Investigator:

DOE is the custodian of several thousand tons of spent nuclear fuel that is intended for geological disposal. The direct disposal of spent nuclear fuel or of mixed oxide fuel (fabricated for the disposal of excess weapons plutonium) requires a careful analysis of the role of spent fuel as a waste form. During burn-up, as much as four percent of the uranium in the fuel will have fissioned to produce stable and radioactive fission products (e.g., Sr, Cs, Tc, I, Mo, Se). In addition, transuranic elements (e.g., Np, Pu, Am, Cm) will have formed from uranium by neutron capture. These radionuclides are cause for concern if they are released in to the biosphere.

In an oxidizing environment, such as in the proposed geological repository at Yucca Mountain, Nevada, rapid alteration rates are expected for spent nuclear fuel, based upon experimental studies of UO_2 and spent nuclear fuel. The alteration involves matrix dissolution of the UO_2 and will release the radionuclides contained within the spent fuel. Researchers in the Chemical Technologies Division of Argonne National Laboratory have ongoing experiments on the oxidative dissolution of both UO_2 and spent nuclear fuel. In both cases, the samples are exposed, by slow dripping in contact with air, to water similar in composition to that found at the Yucca Mountain site. The alteration rate of the UO_2 and spent fuel in the experiments is appreciable, and the alteration products are primarily U^{6+} phases. The generally low concentrations of the fission products and transuranic elements in spent fuel will probably preclude them from forming separate phases. Rather, current research at Argonne National Laboratories indicates that some of these radionuclides are being incorporated into the U^{6+} phases, significantly impacting upon the future mobility of the radionuclides.

We have identified ~20 minerals that contain U^{6+} that are of importance for spent fuel disposal. There is currently inadequate data pertaining to the migration of radionuclides in a repository setting. Only a limited database exists that relates to the effects of alteration phases on the retardation of radionuclides, but this information is necessary in providing a radionuclide release estimate as required for performance assessment modeling. The research will characterize the incorporation of radionuclides into the alteration products, and thus a benefit of our research will be a more realistic estimate of the rate of radionuclide migration from the near field environment. An accurate assessment of realistic radionuclide solubilities in the repository will allow for the development of an effective and cost-efficient engineered barrier system. We will directly study the alteration products of spent nuclear fuel to identify in which phases, and to what extent, the radionuclides of environmental concern are being incorporated. The proposed program of research involves three main components:

1. The structural hierarchy of U^{6+} phases will be applied towards understanding the conditions of formation and regions of stability of U^{6+} minerals, thus allowing the prediction of the types of structural sites for radionuclide incorporation under various physical conditions and chemistries.

2. We will synthesize doped U^{6+} phases and mixed-valence U^{4+}-U^{6+} phases to examine radionuclide incorporation mechanisms. We will verify the types of alteration phases present by comparing with ongoing studies of the alteration of spent fuel at Argonne National Laboratory. These experiments will be done to determine the maximum amount of any given radionuclide that may be incorporated into the structure of each alteration product. Our effort will be focused on those phases found to be important alteration products of spent fuel, as well as other phases that we predict may incorporate radionuclides of interest.

3. We will characterize the radionuclide-doped U^{6+} phases to investigate incorporation mechanisms using X-ray diffraction, analytical transmission electron microscopy, and X-ray Absorption Spectroscopy.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Spent Nuclear Fuel problems, are listed in the <u>Index of High Cost Environmental Management Projects by Problem Area</u>, in the back of this appendix, under the heading "Spent Nuclear Fuel".

Environmental Management Science Program Research in Kansas

University of Kansas

54791-KS - Managing Tight-binding Receptors for New Separations Technologies

Year of Award: 1996 **Amount of Award:** $350,000
Problem Area: Mixed Waste
Science Category/SubCategory: Separations Chemistry / Ligand Design and Ion-exchange
Principal Investigator: Dr. Daryle H. Busch, 913-864-5172, DBusch@caco3.chem.ukans.edu
For More Information: http://www.doe.gov/em52/54791.html

Description Provided by Investigator:

The overall purpose of the chemistry described here is to learn ways in which the most powerful ligands can be made useful in the service of separations science. Advantages of powerful ligands include: metal ions can be taken away from other reasonably strong binding sites, metal ions can be sequestered from very dilute media, and along with high affinity comes the possibility of high selectivity. Historically, the applications of such tight-binding ligands have been limited by the slow rates at which their equilibria are established. This program attacks this limitation in a most basic way, looking at means of facilitating both the binding and release processes, and considering a novel concept for a separations technology that is tolerant of slow equilibration. Three major objectives make up this research: (1) design of tight-binding ligands that can photo-release a metal ion, (2) investigate means for facilitating rapid binding by ligands with very high affinities for selected metal ions, and (3) develop template polymeric receptors that are imprinted for metal complexes of tight-binding ligands, but not for the free ligands. These investigations are motivated by the potential benefits that would derive from bringing extremely tight-binding ligands into separations processes.

Significance

The results sought in the studies would constitute major advances in the fundamental science of coordination chemistry, one of the foundations of separations science. Objective (1) extends the new science of photo-released reagents to metal ions, a development that maybe viewed as overdue. Fundamental questions regarding the photochemical reactions in this research include the following: (1) What will be the effects of the metal ion on the efficiency and, possibly, the nature of the photochemical reaction? (2) What will control the rate of release of the metal ion during the photochemical reaction? In a variety of applications, a metal ion may be firmly chelated until the demand for release is appropriate. At this point, photo release can applied and the metal ion is liberated for whatever role is intended. This could be a part of a separations process, an event in a chemical switching sequence (e.g., signaling the detection of light), the initiation of a metal ion catalyzed process. Thus the possible benefits of the proposed chemistry are wide ranging.

It is extremely important to understand the relationships between the thermodynamic (binding affinities) and kinetic (rates of binding and dissociation) properties of receptor/receptee interactions. This subject is addressed in our objective (2). The affinity of a complex is determined by the ratio of the rates of the binding and dissociation reactions, not the absolute values of those rate processes. Consequently, systems of vastly different labilities can, in principle, exhibit the same affinities. Accumulated knowledge suggests that lability tends to decline as affinity increases, hence the general realization that tight-binding receptors are too slow for traditional separations technologies. There are some hints in the literature of factors that might permit acceleration of the binding process through molecular design. Clarification could lead to many applications because the range of applicable systems would, in many cases, be enhanced.

Objective (3) proposes to extend the varied studies on templated macroporous polymer receptors to the novel role of binding a selected tight-binding complex under conditions appropriate to important applications. These combined studies would also offer strong possibilities of applications and new technologies, or modified and improved technologies. Of particular interest to DOE is the application to the separation of metal ion contaminants from soils and dilute solutions.

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW03	C-287	Mixed Low Level Waste Project
AL024	C-3	Grand Junction Office (GJO) All Other Projects
ID-HLW-101	C-29	High-Level Waste Pretreatment
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ OR-48101	C-99	Offsite Remedial Action
+ OR-45301	C-103	Paducah Remedial Action
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
RL-ER08	C-147	Groundwater Management
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW05	C-173	Process Waste Support
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project
+ SR-HL01	C-249	H-Tank Farm
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Kansas

University of Kansas

54864-KS - Supramolecular Chemistry of Selective Anion Recognition for Anions of Environmental Relevance

Year of Award: 1996 **Amount of Award:** $775,000
Problem Area: Mixed Waste
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Sensors and Techniques
Principal Investigator: Dr. Kristin Bowman-James, 912-864-4673, KBowmanJames@caco3.chem.ukans.edu
Major Collaborator(s): Bruce Moyer at Oak Ridge National Laboratory
For More Information: http://www.doe.gov/em52/54864.html

Description Provided by Investigator:

The supramolecular chemistry of selective anion recognition by synthetic polyammonium macrocycles will be explored in a comprehensive, long term program designed to provide new solutions to problems critical to the environmental initiative of DOE. Highly shape- and charge selective systems will be designed, synthesized, and examined for their capabilities in sequestering environmentally important anions. Phase I of this program (years 1-3) will involve selected oxo anions: nitrate, phosphate, sulfate, chromate, and pertechnetate. Longer term initiatives will include expansion to other environmentally important anions as well as to other non-amine-based receptors. This project will involve major basic research components in the selection of target macrocycles using three areas to assess suitability. These areas are x-ray crystallographic structural determinations, molecular dynamics simulations, and thermodynamic and kinetic studies of anion binding. The results from this basic research component will be applied to environmental challenges including both sensing and separations of anions of interest.

Part I. The basic research components of this project consists of a three-pronged approach, chosen to probe the specifics of anion complexation and to provide a basic comprehensive understanding of anion/cation recognition and interaction.

Solid state structural information obtained by X-ray crystallographic techniques will be obtained to analyze the relationship between positive receptors and negative substrates for oxo anions of environmental interest.

Molecular mechanics and molecular dynamics methodology will be used to aid in the design of improved receptors with enhanced selectivities for anions of interest.

Thermodynamic and kinetic parameters will be used to gauge relative selectivities of the macrocycles for different substrates and will include the determination of protonation constants, complex formation constants, as well as entropies, enthalpies, and free energies of complexation.

Part II. The findings of the basic research component described above will be directed to the selection of receptors to be evaluated in more applied areas in sensor and separations chemistry. These studies will focus on three areas:

The fabrication of anion selective electrodes will be explored at the University of Kansas in our laboratories.

Applications in liquid-liquid separations will be explored in collaboration with Bruce Moyer at Oak Ridge National Laboratory.

The reversible sequestration of heavy metal oxides such a uranyl ion will be examined in collaboration with Paul Smith of Los Alamos National Laboratory. Our role in this project will be to provide appropriate receptors and a summer student to work at the Los Alamos Laboratory.

The results of this comprehensive program can potentially lead to superior systems for sensing and sequestration of anions of environmental importance, and therefore could have majorimpact on issues involving hazardous waste sources, including Hanford underground tanks, groundwater, and process waste waters.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW03	C-287	Mixed Low Level Waste Project
NV214	C-53	Industrial Sites
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Kansas

University of Kansas

60199-KS - Seismic-Reflection and Ground Penetrating Radar for Environmental Site Characterization

Year of Award: 1997 **Amount of Award:** $630,000
Problem Area: Remedial Action
Science Category/SubCategory: Geophysics / Subsurface Imaging
Principal Investigator: Dr. Don W. Steeples, 913-864-2730, steeples@kuhub.cc.ukans.edu
For More Information: http://www.doe.gov/em52/60199.html

Description Provided by Investigator:

This research seeks to show how shallow, high-resolution, three-component seismic reflection techniques, in concert with ground-penetrating radar (GPR), might assist in characterizing hydrologic-transport parameters at environmentally sensitive sites. The high dynamic range and many channels typical of modern seismographs, along with advances in ground-penetrating radar technology, offer more opportunities than ever before to extract useful information from the subsurface. Both techniques are noninvasive and can be used in situ. Combined, they offer the prospect of improved near-surface imaging with minimal environmental impact. Furthermore, shallow, three-component seismology and GPR have not been used together to examine the same volume of shallow earth in this manner before.

Landfills, industrial plants, mine-waste dumps, and chemical spills are widespread in the United States, and they have the potential to introduce significant levels of leachates into local and regional aquifers. Establishing the spatial extent of the contamination as well as identifying the transport-flow directions and fates of the contaminants are essential to developing safe, effective, and cost-sensitive remediation strategies. Yet tracing preferential permeability paths in sufficient detail to allow quantitative analysis is among the most challenging problems currently facing hydrologists. Some of the factors limiting the accuracy of hydrologic predictions are lateral heterogeneity, unexpected stratigraphic layering, fracturing, and flow anisotropy. Commonly, our knowledge of these controlling hydrologic factors is derived from conceptual knowledge of regional geology coupled with information derived from drilling. However, invasive processes such as drilling are time consuming, costly, and can exacerbate existing problems. Furthermore, the information obtained from them is point-specific and may not provide the detail needed about the region between drilled holes. A combined seismic/GPR imaging approach has the potential to offer a low-impact, cost-effective alternative at some sites.

Accordingly, the goals of the research are (1) to examine the complementary site-characterization capabilities of modern, three-component, shallow-seismic reflection and GPR methods at depths ranging between 2 and 8 m, (2) to demonstrate the usefulness of the combined methods to characterize the three-dimensional shape of the cone of depression around a pumping well and monitor for anisotropic flow, and (3) to allow the site to function as an outdoor mesoscale laboratory to validate existing three-dimensional ground-penetrating radar and seismic-reflection computer models developed at the University of Kansas.

To accomplish these goals, a 120-channel, 24-bit seismograph will be used to collect the seismic data, and a Pulse EKKO 1000 ground-penetrating radar equipped with a high-speed data-acquisition subsystem will be used to obtain the radar data. The test site to be used has produced P-wave seismic-reflection data of exceptional quality previously, obtained at depths as shallow as 2.6 m. Ground-penetrating radar data collected recently at this location are of high quality as well. The test site has attributes that are particularly useful for this research, and, although itself uncontaminated, the location is well-suited to serve as a proxy site for existing contaminated areas.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV212	C-49	Underground Test Area (UGTA)
§ NV214	C-53	Industrial Sites
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER02	C-129	200 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ RF014	C-213	Industrial Zone Closure Project
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project

Environmental Management Science Program Research in Louisiana

Tulane University

55032-LA - Environmental Analysis of Endocrine Disrupting Effects from Hydrocarbon Contaminants in the Ecosystem

Year of Award: 1996 **Amount of Award:** $619,995
Problem Area: Health / Ecology / Risk
Science Category/SubCategory: Health Science / Health Effects
Principal Investigator: Dr. John McLachlan, 504-585-6910, jmclach@mailhost.tcs.tulane.edu
Major Collaborator(s): Dr. Ann Cheek at Tulane University
For More Information: http://www.doe.gov/em52/55032.html

Description Provided by Investigator:

RESEARCH OBJECTIVE

The objective of this basic research is to characterize the potential of common hydrocarbon contaminants in ecosystems to act as endocrine disrupters. Although the endocrine disrupting effects of contaminants such as dioxin and PCBs have been well characterized in both animals and humans, little is known about the capacities of other hydrocarbon contaminants to act as endocrine disrupters. One of the most promising approaches to the problem of characterizing endocrine disruption caused by environmental contaminants --endocrine activation in yeast cells-- resides at the Tulane/Xavier Center for Bioenvironmental Research.

BACKGROUND

Similar hydrocarbon contaminants are present at DOE sites and at oil and gas related sites in Louisiana. DOE National Laboratory sites (e.g., Savannah River Site, A/M Area, SC), DOD sites (e.g., McClellan Air Force Base, Operable Unit B/C, CA), and EPA Superfund sites (e.g., French Ltd. Superfund Site, TX) are contaminated with mixtures of semivolatile polynuclear aromatic hydrocarbons, other chlorinated and non-chlorinated hydrocarbons, and in some cases, dioxins, PCBs, and pesticides. Ongoing remediation projects include removal of hydrocarbon contaminants from soil, sludge, groundwater, and sediments using conventional pump & treat methods. Similarly, Bayou Trepagnier and other sites in the state of Louisiana, contaminated by past oil and gas refining activities, contain a variety of similar hydrocarbon contaminants. Working under an initial grant from the DOE, the Tulane/Xavier Center for Bioenvironmental Research (CBR) has characterized hydrocarbon contamination in sediments in Bayou Trepagnier where 14/20 sample sites along the Bayou contain hydrocarbon contaminants at levels that correlate with moderate to high adverse effects related to standard ecotoxicity and animal toxicity endpoints.

Clean-up levels related to hydrocarbon contaminants at DOE sites have been based on conventional quantitative risk assessments that consider toxicity, dose, exposure duration and pathways, as well as induced health effects. As a result of the DOE Draft 1995 Risk Report to Congress, the sites are being made aware of the need to determine risks to humans, the environment, and ecosystems and to identify and describe individual populations or segments of the environment that would be at risk from the hazards that are present at the sites. The Proposed Guidelines to revise EPA's 1986 Guidelines for Carcinogen Risk Assessment attempt to address the limitations of the 1986 Guidelines where identification of potential human hazard relied heavily on tumor findings, and in practice, seldom made full use of all biological information.

New data indicate that low levels of hydrocarbon contaminants may represent even greater sources of risk to ecosystems and to human health by acting as endocrine disrupters. Since the 1940's, ecological data have indicated that hydrocarbons placed in the environment byagricultural and industrial activities can have profound effects on the health and fitness of whole animal populations including eagles, otters, seabirds, and alligators. Most of the adverse effects were attributed to disruption by hydrocarbon contaminants of normal endocrine activities in these animals. For example, spills of industrial contaminants into Lake Apopka in Florida not only reduced the natural alligator population dramatically, but also feminized male alligators that remained. In addition, laboratory data indicated that specific contaminants that act as false estrogens such as PCBs and dioxins can influence mammalian reproductive development and development of the nervous system. Studies on fish consumption by pregnant mothers in the Great Lakes region and in North Carolina unequivocally showed that exposure to these compounds produce dramatic alterations in cognitive abilities in children exposed during gestation. There is also evidence that human sperm concentrations have declined in males growing up in industrial settings since 1930.

In all cases, toxicity is thought to be caused by exposure to environmental contaminants acting as endocrine disrupters, that is, serving as false hormones. The contaminants bind natural hormone receptors, over-activating endocrine cells, or activating them at the wrong time, or the contaminants block hormone receptors, shielding them from interacting with appropriate natural hormones. This new class of toxic disruption is of extreme interest to the regulatory and scientific community because risk assessments related to clean-up efforts do not factor endocrine disrupting effects into risk analysis. Thus, clean-up at DOE National Laboratory sites, DOD sites, and industrial and Superfund sites, may be compromised due to failure to remove contaminants to appropriate low levels that would preclude endocrine disruptive effects.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Health / Ecology / Risk problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Health / Ecology / Risk".

Environmental Management Science Program Research in Maine

University of Maine

55071-ME - Reduction and Immobilization of Radionuclides and Toxic Metal Ions Using Combined Zero Valent Iron and Anaerobic Bacteria

Year of Award: 1996 **Amount of Award:** $356,089
Problem Area: Remedial Action
Science Category/SubCategory: Biogeochemistry / Biogeochemistry
Principal Investigator: Dr. Lenly Weathers, 207-581-2171
For More Information: http://www.doe.gov/em52/55071.html

Description Provided by Investigator:

Large groundwater plumes contaminated with toxic metal ions, including radionuclides, exist at several DOE facilities. Previous research indicated that both zero valent iron and sulfate reducing bacteria can yield significant decreases in concentrations of redox sensitive metals and radionuclides due to abiotic and biotic reduction, respectively. The major hypothesis of this research is that a combined abiotic-biological system can synergistically combine both processes to maximize metal ion reduction in an engineered permeable reactive barrier. The second major hypothesis is that design of either in situ or ex situ metal ion reduction processed based on biotic, abiotic or combined abiotic/biotic reduction scheme requires a more thorough understanding of the rates of the reaction and quantification of the parameters which impact the rates of reduction. A natural corollary to this hypothesis is that this increased understanding must also include quantification of parameters or parameter levels which inhibit either the biotic and abiotic process. The overall goal of this project is to design a combined abiotic/biotic, reactive, permeable, in situ barrier with sufficient reductive potential to prevent downgradient migration of toxic metal ions. Successful completion of this goal required evaluating (1) the kinetics of abiotic metal ion reduction under a range of environmental conditions and (2) the kinetics of biotic processes under a range of environmental conditions.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

Environmental Management Science Program Research in Maryland

National Institute of Standards &Technology - Maryland

60231-MD - Novel Miniature Spectrometer for Remote Chemical Detection

Year of Award: 1997 **Amount of Award:** $549,000
Problem Area: Mixed Waste
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Sensors and Techniques
Principal Investigator: Dr. Jeffrey W. Hudgens, 301-975-2512, Hudgens@NIST.gov
For More Information: http://www.doe.gov/em52/60231.html

Description Provided by Investigator:

This research will develop an entirely new class of chemical sensing technology that will enable qualitative and quantitative remote, real-time diagnostics of chemical species in hazardous gas, liquid, and semi-solid phases through a completely novel implementation of evanescent wave spectroscopy. The sensor design utilizes a small, solid block (< $1 cm^3$) of ultra-high purity optical material that is fabricated into a regular, planar polygon with a convex facet to form a total-internal-reflection ring cavity. For light undergoing sustained circulation by total-internal-reflection inside the solid, the facets of the polygon act as extremely high-reflectivity (99.9999% in some cases) mirrors, resulting in a relatively long and accurately measurable lifetime for an injected light pulse. Evanescent waves, which are generated by total-internal-reflection, are absorbed by matter in the vicinity of the cavity where the evanescent wave decays exponentially in space. The absorption spectrum is extracted by measuring the mean lifetime of an injected light pulse as a function of pulse carrier frequency. Errors associated with light source fluctuations, which typically limit the sensitivity of conventional absorption methods, are eliminated by this single pulse measurement, as in the gas-phase technique known as cavity ring-down spectroscopy. By locating the light source and detection system at a distance (e.g., 0.1 to 10 Km) through the use of fiber-optics, this new technology will permit remote, high-sensitivity, broadband chemical sensing with a rugged, cost-effective, miniature spectrometer.

Preliminary studies indicate the feasibility and design considerations for this new class of devices. For the laboratory program the technical tasks include: 1) experiments that verify chemical sensitivity, 2) development of a fabrication strategy for ruggedly mounting the coupling prisms to the TIR-ring cavity, 3) design and fabrication of TIR-ring cavities that allow detection of chemical species in the near-and mid-infrared (IR) spectrum, 4) development of a fiber-optic interface to TIR-ring cavities, 5) characterization of the technology by using these devices to detect chemical species of importance to the EMSP mission, and 6) investigation of potential interferences, e.g., particulates, abrasives, inhomgeneities, temperature and density gradients.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§ ID-WM-107	C-45	Long Term Treatment/Storage/Disposal Operations
§ RL-WM03	C-193	Solid Waste Storage and Disposal
§ RL-WM04	C-197	Solid Waste Treatment
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW02	C-285	Transuranic Waste Project
§+ SR-SW03	C-287	Mixed Low Level Waste Project
AL007	C-7	Environmental Restoration
+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
ID-HLW-101	C-29	High-Level Waste Pretreatment
NV212	C-49	Underground Test Area (UGTA)
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
OR-43204	C-77	ORNL Bethel Valley Deactivation and Decommissioning
+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ OR-45301	C-103	Paducah Remedial Action
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
RL-ER08	C-147	Groundwater Management
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW04	C-169	Retrieval Project
+ RL-TW05	C-173	Process Waste Support
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project
+ SR-HL01	C-249	H-Tank Farm
+ SR-HL02	C-253	F-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Maryland

Uniformed Services University of the Health Sciences

59786-MD - Design and Construction of Deinococcus radiodurans for Biodegradation of Organic Toxins at Radioactive DOE Waste Sites

Year of Award: 1997 **Amount of Award:** $799,997
Problem Area: Remedial Action
Science Category/SubCategory: Microbial Science / Microbial Genetics and Instrumentation
Principal Investigator: Dr. Michael J. Daly, 301-295-3750, mdaly@USUHS.MIL
Major Collaborator(s): James K. Fredrickson at Pacific Northwest National Laboratory
Lawrence P. Wackett at the University of Minnesota
For More Information: http://www.doe.gov/em52/59786.html

Description Provided by Investigator:

A 1992 survey of DOE waste sites indicates that about 32% of soils and 45% of groundwaters at these sites contain radionuclides and metals plus an organic toxin class. The most commonly reported combinations of these hazardous compounds being radionuclides and metals (e.g. U, Pu, Cs, Pb, Cr, As) plus chlorinated hydrocarbons (e.g., trichlorethylene), fuel hydrocarbons (e.g., toluene), or polychlorinated biphenyls (e.g., Arochlor 1248). These wastes are some of the most hazardous pollutants and pose an increasing risk to human health as they leach into the environment.

This research is a collaborative project under development since June 1996 that brings together the experience of three diverse laboratories to develop a cost-effective new technology that targets the organic toxins, at radioactive waste sites, for complete degradation. The objective of this research is to develop novel organisms, that are highly resistant to radiation and the toxic effects of metals and radionuclides, for in situ bioremediation of organic toxins. The soil bacterium we have been using is *Deinococcus radiodurans*, the most radiation resistant organism discovered to date. *D. radiodurans* is also highly resistant to the effects of desiccation, the mutagenic effects of UV radiation, most chemical DNA damaging agents and, as we show here, is resistant to the effects of organic solvents. We have successfully tested our research strategy showing that catabolic genes from other bacteria can be expressed in *D. radiodurans*, even in highly radioactive conditions (60 Gy /hour). Other bacteria that are known to degrade organic toxins are relatively radiation sensitive-rendering their bioremediating genes useless in radioactive environments. As a result of our work on developing *D. radiodurans* for bioremediation, *in situ* biodegradation of the organic components of radioactive sites has become a realistic goal.

The strategies we describe for engineering bioremediating *D. radiodurans* strains are built on results presented here showing the degradation of toluene, chlorobenzene, dichlorobutene and indole by genetically engineered *D. radiodurans*, in the presence and absence of radiation. Our aim is to engineer strains of *D. radiodurans* that can: 1) degrade and utilize the organic toxins as energy and carbon sources; and 2) survive the toxic effects of the co-contaminating metals. By using the organic toxins as carbon sources, *D. radiodurans* strains may not require *in situ* stimulation for toxin degradation, but instead would be able to generate energy necessary to sustain growth by metabolizing the organics.

Our large collection of *D. radiodurans* vectors will be used to test genes for toxin degradation as well as metal resistance, alone or in combination. Toxin-degrading gene expression levels in *D. radiodurans* will be optimized using a variety of expression vectors and each novel strain will be characterized for intermediate and terminal metabolites of organic toxin degradation as well as for metal resistance activity. This research will provide radiation-resistant bacteria with considerable potential for *in situ* and *ex situ* remediation of organic toxins at high-radiation, high-toxicity DOE sites.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§ RL-ER08	C-147	Groundwater Management
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Maryland

Johns Hopkins University Applied Physics Lab

59977-MD - Synthesis and Characterization of Templated Ion Exchange Resins for the Selective Complexation of Actinide Ions

Year of Award: 1997 **Amount of Award:** $302,047
Problem Area: High Level Waste
Science Category/SubCategory: Actinide Chemistry / Actinide (Heavy Element) Chemistry
Principal Investigator: Dr. George M. Murray, 410-792-6000 ext. 3882, murragm1@aplcomm.jhuapl.edu
For More Information: http://www.doe.gov/em52/59977.html

Description Provided by Investigator:

Current technologies for the production and handling of the actinides produce significant environmental impacts at existing sites. Leaks and leachings of wastes from tanks, resulting in contamination of the environment, can result in expensive clean up procedures. Normal methods of separation are unable to cope with the problem of clean up on such a large scale due primarily to a lack of selectivity. Many Department of Energy sites and facilities have been contaminated by a variety of metal wastes. Since a large fraction of these wastes are already in aqueous solution or are water soluble, this source of contamination needs to be assessed and remediated. To perform the required assessment and remediation with currently available technologies would create huge quantities of waste and would environmentally impact the site itself. New technologies are needed immediately to allow for rapid, compact and less costly assessment. Further, its use for remediation should not result in large quantities of waste in need of further clean-up and disposal. An ideal new technology would quickly provide assessment tools and provide a means of reclamation of the wastes by converting these wastes to valuable raw materials. The emerging technology being proposed here will provide these benefits by the application of metal ion templated polymers for the selective sensing and sequestering of uranyl and other actinide ions.

The purpose of this research is to develop a polymeric extractant for the selective complexation of uranyl ions (and subsequently other actinyl and actinide ions) from aqueous solutions (lakes, streams, waste tanks and even body fluids). Chemical insights into what makes a good complexation site will be used to synthesize reagents tailor-made for the complexation of uranyl and other actinide ions. These insights, derived from studies of molecular recognition include ion coordination number and geometry, ionic size and ionic shape, as well as ion to ligand thermodynamic affinity.

Selectivity for a specific actinide ion will be obtained by providing the polymers with cavities lined with complexing ligands so arranged as to match the charge, coordination number, coordination geometry, and size of the actinide metal ion. These cavity-containing polymers will be produced by using a specific ion (or surrogate) as a template around which monomeric complexing ligands will be polymerized. The complexing ligands will be ones containing functional groups known to form stable complexes with a specific ion and less stable complexes with other cations. Prior investigator's approaches for making templated resins for metal ions have had marginal success. We have extended and amended these methodologies in our work with Pb(II) and uranyl ion, by changing the order of the steps, by the inclusion of sonication, by using higher complex loading, and the selection of functional groups with better complexation constants. This has resulted in significant improvements to selectivity. The unusual shape of the uranyl ion suggests that this approach will result in even greater selectivities than already observed for Pb(II). Preliminary data obtained for uranyl templated polymers shows unprecedented selectivity and has resulted in the first ion selective electrode for uranyl ion.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§+ RL-TW04	C-169	Retrieval Project
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§+ SR-HL01	C-249	H-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
§ SR-HL05	C-265	Vitrification
AL024	C-3	Grand Junction Office (GJO) All Other Projects
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ OR-48101	C-99	Offsite Remedial Action
+ OR-45301	C-103	Paducah Remedial Action
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
RL-ER08	C-147	Groundwater Management
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Maryland

University of Maryland

55152-MD - Molecular Profiling of Microbial Communities from Contaminated Sources: Use of Subtractive Cloning Methods and rDNA Spacer Sequences

Year of Award: 1996 **Amount of Award:** $607,021
Problem Area: Remedial Action
Science Category/SubCategory: Microbial Science / Microbial Genetics and Instrumentation
Principal Investigator: Dr. Frank T. Robb, 410-234-8803, robb@umbi.umd.edu
For More Information: http://www.doe.gov/em52/55152.html

Description Provided by Investigator:

This research addresses the development and testing of molecular methods that will allow rapid characterization of microbial communities in perturbed or contaminated ecosystems. The major objective of the research is to provide appropriate sequences and to assemble a high-density DNA array (Biochip) of oligonucleotides that can be used for rapid profiling of microbial opulations from polluted areas. The sequences to be assigned to the DNA array will be chosen from cloned genomic DNA from DOE mixed-waste sites containing chlorinated and unchlorinated organic solvents and heavy metals. We have well characterized pollutant histories assembled by our collaborators at the PNL. Pristine analog sites are available for the areas, and the proposed objective is to develop rapid monitoring capability for the microbial populations present at each site.

The development of a large sequence database of ribosomal RNA intergenic spacer regions (ISRs) and sequences derived from subtractive cloning methods will reflect genetic selection at the contaminated sites. Collection of the sequences will utilize our prior experience in microbial genomic research, and in amplifying and sequencing the ISR, a relatively variable region flanked by conserved priming sites in the 16S and 23SrDNA regions. ISR sequences have been used recently in our laboratory to distinguish closely related hyperthermophilic strains but they have not yet been used in defining natural microbial populations, mainly because of the lack of a comprehensive sequence database. The generation of subtractive libraries will reflect the genomic DNA sequences, including the spacer regions, that are restricted to either the pristine or polluted sites. The sequences obtained from these studies will allow the design of DNA probe arrays that will detect and identify bacteria at genus level, and will allow a quantitative assessment of the key physiological traits represented in the population. The rapid acquisition of microbial genomic DNA sequences as a result of the acceleration of microbial genome sequencing activities will permit extensive gene discovery as an additional product of the research.

Proein-encoding genomic sequences from populations in contaminated sites will enable the use of conserved sequences for detection of strains with degradative or metal-resistance genes. This could allow sensitive detection of genes related to the pollution history of polluted sites and the progression of degradation, and bring this method of detection into more general use in bioremediation.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§ RL-ER08	C-147	Groundwater Management
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Massachusetts

Woods Hole Oceanographic Institute

54683-MA - Speciation and Structural Characterization of Plutonium and Actinide-organic Complexes in Surface and Groundwaters

Year of Award: 1996 **Amount of Award:** $823,481
Problem Area: Remedial Action
Science Category/SubCategory: Actinide Chemistry / Actinide (Heavy Element) Chemistry
Principal Investigator: Dr. Ken O. Buesseler, 508-289-2309, kbuessel@nsf.gov
Major Collaborator(s): Dr. James M. Kelley at Pacific Northwest National Laboratory
Dr. Daniel J. Repeta at Woods Hole Oceanographic Institute
For More Information: http://www.doe.gov/em52/54683.html

Description Provided by Investigator:

We are studying the chemical nature of the actinides and their association with specific organic ligands in the natural environment. We will bring to this study a range of newly developed technologies which the PI's have used to study the physical organic and structural features of dissolved organic matter (DOM) and the association of trace metals and radionuclides with the particulate, colloidal and dissolved phases. The application of cross-flow ultrafiltration (CFU) techniques will allow us to quantitatively recover DOM from surface and groundwater, and separate it without significant loss into different size classes, ranging from 1 kilo-Dalton (kD) to 100 kD (e.g. Buffle *et al.*, 1992). Given such samples, we can thus assess for each fraction the total colloidal actinide binding activity, but more importantly, we will isolate, purify, and structurally characterize actinide-binding polymers in natural waters. The application of thermal ionization mass spectrometry (TIMS) is essential for the detection of Pu, Np and U for this study. Most importantly, TIMS will provide: a) the sensitivity needed to make these measurements on small samples at ambient fallout levels and in the far field migration of groundwater actinides; b) the ability to use isotope ratios to distinguish between fallout and other possible sources; and c) will allow us to compare the *in-situ* behavior of a suite of actinides with similar sources but differing environmental geochemistries (Buesseler and Halverson, 1987; Stoffel *et al.*, 1994).

Conceptual and analytical advances made over the last decade have significantly altered our view of DOM in aquatic systems and the approach taken to study actinide-organic complexation. The traditional view that actinide-organic matter complexation is primarily with humic substances may be incorrect. Non-humic DOM may support much of the actinide binding activity of colloids. DOM may not be a poorly structured assembly of random polymers, but may include a large fraction of highly ordered biopolymers. The sites to be chosen for study therefore span a range of DOM characteristics and redox settings. Given the labor intensity of the analyses we would focus on a limited range of sites, but a wide range of geochemistries. We would optimize our sampling and analytical strategies during the first year using samples from organic-rich fresh water ponds in the Woods Hole area. Subsequent field trips (one in each of years 2 and 3) would be conducted to sites where there is contrasting geochemistry's for study and some concern about migration of actinides from waste sources. One proposed site is at the Savannah River Facility, where a previous study of monitoring wells adjacent to an unlined seepage basin, suggests that Pu(IV) organic colloids have migrated much more rapidly than predicted (> 1 km- Kaplan *et al.*, 1994). Finally, we will also sample subsurface waters from the Hanford Reservation with assistance from our colleagues from Pacific Northwest Lab (PNL). This will allow for a comparison of actinide speciation between surface and sub-surface waters and permit us to examine the relative transport of Pu originating from global fallout and waste related sources (separated via TIMS isotopic analyses).

Once collected, samples would be split. Total radionuclide, organic and supporting geochemical measurements, and CFU processing would be conducted in the field for isolation of the colloidal size-classes. For the radionuclides, we would measure not only total concentration using TIMS analyses, but also perform redox separations to determine for example, the relative abundance of the more oxidized or reduced forms of Pu in the colloidal vs. ultrafiltrate size-classes. Ofparticular interest is how the redox chemistry of Pu varies as a function of ambient DOM levels and site specific characteristics. The structural characteristics of the DOM will be determined using a range of techniques, including 2-D NMR, high resolution electrospray MS/MS, and pyrolysis-GC/isotope ratio MS. An important feature of this approach is that we can then integrate information on molecular composition (simple sugars, amino acids and lipids, etc.) with information on polymer structure (Aluwihare *et al.*, 1996). The importance of understanding the macromolecular features of DOM cannot be over emphasized. Previous models which have treated colloidal organic matter as a single phase or have limited chemical characterization to humic substances only, have not been successful in describing metal binding activity and physical chemical characteristics of DOM.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ AL007	C-7	Environmental Restoration
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV212	C-49	Underground Test Area (UGTA)
§ NV214	C-53	Industrial Sites
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER02	C-129	200 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Massachusetts

Massachusetts Institute of Technology

54888-MA - Manipulating Subsurface Colloids to Enhance Cleanups of DOE Waste Sites

Year of Award: 1996 **Amount of Award:** $451,421
Problem Area: Remedial Action
Science Category/SubCategory: Hydrogeology / Fluid-flow and Colloidal Dynamics
Principal Investigator: Dr. Philip M. Gschwend, 617-253-1638, pmgschwe@MIT.EDU
For More Information: http://www.doe.gov/em52/54888.html

Description Provided by Investigator:

Colloidal phases, such as submicrometer iron oxyhydroxides, aluminosilicate clays, and humic macromolecules, are important subsurface sorbents for the low-solubility chemicals in DOE wastes. Recent research we have performed as part of DOE's Subsurface Science Program has demonstrated that such colloid-sized media may be mobilized in groundwater under certain conditions and thereby may enhance the below-ground transport of sorbed contaminants. This "colloid facilitated transport" may be problematic if it results in unwanted spreading of groundwater contaminants, but it may be beneficial if it can be controlled and used in efforts to remove low-solubility chemicals from the subsurface. At the present, in but a few cases, we do not know the basic mechanisms responsible for holding colloids immobile in aquifers. Further, we are lacking fundamental understandings of the processes involved in detaching colloids from these geological media as a result of planned or unplanned changes in the groundwater solution chemistry.

This research project seeks to improve these basic understandings in a manner which should improve DOE's ability to control and remediate the existing legacy of waste sites. First we propose to observe directly the particle:particle associations holding colloids immobile in several characteristic aquifer sands. These aquifer solids will be recovered (1) from a geological sequence of iron oxyhydroxide-coated beach deposit aquifers extending inland from the coast of South Carolina, and (2) a north-south sample series from representative deposits located in Connecticut (glacial outwash), New Jersey (northern coastal plain), as well as South Carolina (southern coastal plain).

Next, we will test our ability to mobilize colloids from these sands in the laboratory using aqueous solutions of appropriate composition (e.g., low pH, low ionic strength, surfactant amended) suggested by our observations of particle:particle attachments. We will also investigate the solid-solution interactions that limit our ability to impose particular solution conditions.

Finally, we will purposefully mobilize the colloids at a chromium-contaminated field site (the glacial outwash site in Connecticut noted above) to ascertain the importance of field properties such as heterogeneous flow paths.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ AL024	C-3	Grand Junction Office (GJO) All Other Projects
§ NV214	C-53	Industrial Sites
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ OR-48101	C-99	Offsite Remedial Action
§+ OR-45301	C-103	Paducah Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ RF014	C-213	Industrial Zone Closure Project
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Massachusetts

Massachusetts Institute of Technology

55141-MA - Imaging and Characterizing the Waste Materials Inside an Underground Storage Tank Using Seismic Normal Modes

Year of Award: 1996 **Amount of Award:** $575,703
Problem Area: High Level Waste
Science Category/SubCategory: Geophysics / Subsurface Imaging
Principal Investigator: Dr. M. Nafi Toksöz, 617-253-7852, nafi@ERL.MIT.EDU
For More Information: http://www.doe.gov/em52/55141.html

Description Provided by Investigator:

The objective of this study is to develop and test a seismic method to image and characterize waste materials contained in tanks using complete seismic response including the normal modes, or "free oscillations." The method will be developed with the ultimate application to image and characterize waste materials inside the large underground storage tanks at Hanford. Obtaining seismic parameters inside the tanks would help define the material properties, such as the layering, fraction of solid and liquid phase, and the presence of interstitial gas in the material, since these could be inferred from seismic velocities and attenuations. This study includes three major tasks.

1. Calculate theoretically the seismic response of a partially filled tank with sources located inside the tank and outside the tank and receivers inside the tank. Analyze these synthetic responses to identify the normal mode peaks. Match the synthetic responses with the properties of the layered material inside the tank.

2. Test the method in the laboratory using a 100 to 1 scaling of the Hanford tanks with a corresponding scaling of wavelengths. Make measurements in the laboratory to study various important aspects of the problem such as the sensitivity of the method to various parameters, including source location, layering, velocity contrasts, and elastic and inelastic material properties.

3. Conduct a full-scale feasibility experiment at Hanford. Place hydrophone strings in one or more tanks and place the source on the surface outside the tank. If the source outside the tank works, as predicted by the preliminary calculations, this could provide a safe and efficient seismic method for determining material properties inside the tank.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

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"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§+ RL-TW04	C-169	Retrieval Project
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations

Environmental Management Science Program Research in Massachusetts

Massachusetts Institute of Technology

55300-MA - 3-D Spectral IP Imaging: Non-Invasive Characterization of Contaminant Plumes

Year of Award: 1996 **Amount of Award:** $710,097
Problem Area: Remedial Action
Science Category/SubCategory: Geophysics / Subsurface Imaging
Principal Investigator: Dr. F. Dale Morgan, 617-253-7857, morgan@erl.mit.edu
Major Collaborator(s): David Lesmes at Boston College
For More Information: http://www.doe.gov/em52/55300.html

Description Provided by Investigator:

The objective of this study is to develop a *noninvasive tomographic imaging technique,* based on the *spectral induced-polarization method,* to characterize the *in-situ distribution of organic and inorganic groundwater contaminants.* Recent advances in tomographic imaging, applied to d.c. resistivity data have made it possible and practical to obtain high-resolution 3-D images of sub surface resistivity structures. However, imaging of contaminant plumes with the d.c. resistivity method is only feasible in cases where the level of contamination is relatively high. Alternatively, the spectral IP response of rocks and soils, which arises from the polarization of an electrochemical surface phase at grain-solution boundaries, is very sensitive to even small amounts of contaminants. We plan to further develop our d.c. resistivity tomographic imaging algorithms to obtain a 3-D inversion code for spectral IP data. The resulting 3-D map of the spectral IP response can be used to characterize the subsurface chemical conditions. Laboratory studies will be conducted with the goal of obtaining a quantitative interpretation of the derived IP spectra in terms of the contaminant type and concentration. Lastly, field studies will be conducted at well-characterized field sites to test the overall performance of this integrated imaging method and to test new developments in field instrumentation. If this remote sensing method proves successful it will greatly enhance our ability to detect, identify, and map the distribution of contaminants in the subsurface. This technology will provide tremendous cost savings in terms of the number of boreholes that are necessary to characterize a contaminated site and it will be extremely useful in the characterization and monitoring of in-situ chemistry for remediation efforts.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV212	C-49	Underground Test Area (UGTA)
§ NV214	C-53	Industrial Sites
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER02	C-129	200 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation

Environmental Management Science Program Research in Massachusetts

Northeastern University

54571-MA - Removal of Heavy Metals and Organic Contaminants from Aqueous Streams by Novel Filtration Methods

Year of Award: 1996 **Amount of Award:** $330,000
Problem Area: Mixed Waste
Science Category/SubCategory: Separations Chemistry / Ligand Design and Ion-exchange
Principal Investigator: Dr. Nelly M. Rodriguez, 617-373-2085, n.rodriguez@nunet.neu.edu
For More Information: http://www.doe.gov/em52/54571.html

Description Provided by Investigator:

Catalytically grown carbon nanofibers are a novel material that is produced by the decomposition of selected hydrocarbons over metal particles. The material consists of graphite platelets perfectly aligned and stacked in various directions with respect to the fiber axis. Such an arrangement imparts the carbon nanofibers with a unique combination of physical and chemical properties, including a high electrical conductivity. Perhaps one of the most unexpected findings is that such extraordinarily ordered crystalline solids can exhibit high surface areas, typically ~ 300 m^2/g as grown, which can be enhanced to about 700 m^2/g. Furthermore, by choice of the catalyst and reaction conditions it is also possible to generate structures with different spacing between the platelets, thereby generating new types of sieves. We have developed a process by which it is possible to produce large amounts of nanofibers at the laboratory level, and it is estimated that on a large scale this material could be produced at a cost of ~$1.50/lb, about a tenth of the cost of commercial graphite.

In one section of the program high surface area electrically conductive carbon nanofibers will be employed as the electrode material in the fabrication of unique types of electrochemical filtration and selective collection devices to be used for the removal of heavy metals, radionuclides and transuranic elements from liquid phase effluent streams. Preliminary studies conducted with highly graphitic carbon nanofibers have indicated that the material exhibits a superior performance for the removal of metal ions from low concentration solutions when used as an electrode in an electrochemical cell over that displayed by graphite felts, metal mesh and other forms of conductive carbon. Furthermore, by application of a reverse potential, the metal species that are bound on the nanofiber surface can be rapidly released into a more concentrated solution for eventual recovery or disposal. Having demonstrated the feasibility of this concept for the removal of cadmium, lead and copper species from aqueous solutions both by electroplating and electrosorption methods, we now plan to optimize the performance of the electrode for the removal of metals that are of major concern in the waste streams existing at numerous nuclear production and processing sites. In a complementary series of electrochemical studies the influence of such factors as solution flow rate through the nanofiber bed, variations in bed height and pH of the contaminant solution will be addressed. In this section of the work, efforts will be focused on the removal and collection of such metals as uranium, plutonium, cesium, radium, thorium and strontium.

In a further portion of the project we intend to take advantage of the unique blend of properties of carbon nanofibers for the separation of organic residues including, methylene chloride, tetrahydrofuran, chlorobenzene, toluene, and methylethylketone, from water streams. The approach takes into account the presence of the graphite platelets, that are stacked in a similar manner to a pack of cards, with a minimum interlayer spacing of 0.34 nm that can be expanded by at least 20% without loss of structural integrity. It is anticipated that the organic molecules with be preferentially drawn into the interlayer structure of the nanofibers because of the establishment of a strong interaction of such species with the non-polar basal plane regions of the graphite platelets. We shall also exploit the flexibility of carbon materials with regard to the ability to modify their functionality by suitable treatments. In the present case such treatments will result in a change in polarity of the edge regions of the graphite platelets leading to anenhancement in the wetting of the carbon by the aqueous phase without interfering with the adsorption characteristics of the organic constituent. If desired, the organic compound can be recovered by desorption.

These fundamental studies will provide the rudiments for a large scale process where it is envisioned that removal of organic contaminants from an aqueous stream will be carried out by direct adsorption in the interlayer spaces of the carbon nanofibers in the first stage. Following this step, trace metallic impurities will be trapped on the active edge sites of nanofibers in a series of electrochemical filtration devices. This operation will be achieved by controlled cathode potentials, where increasing negative potentials are applied to a series of carbon nanofiber electrodes and this arrangement functions in a similar manner to a chromatographic column. The sequential application of reverse potentials will then enable each component to be recovered in the "pure" state. This would be an ideal method for purification of contaminated ground water, allowing for the separation of such contaminants as calcium, lead and radionuclides.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW03	C-287	Mixed Low Level Waste Project
+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
ID-HLW-101	C-29	High-Level Waste Pretreatment
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ OR-48101	C-99	Offsite Remedial Action
+ OR-46301	C-107	Portsmouth Remedial Action
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
RL-ER08	C-147	Groundwater Management
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW05	C-173	Process Waste Support
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project
+ SR-HL01	C-249	H-Tank Farm
+ SR-HL02	C-253	F-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Michigan

Michigan State University

55105-MI - Complete Detoxification of Short Chain Chlorinated Aliphatics: Isolation of Halorespiring Organisms and Biochemical Studies of the Dehalogenating Enzyme Systems

Year of Award: 1996 **Amount of Award:** $196,056
Problem Area: Remedial Action
Science Category/SubCategory: Microbial Science / Biodegradation and Biotransformation
Principal Investigator: Dr. James M. Tiedje, 517-353-9021, tiedjej@pilot.msu.edu
For More Information: http://www.doe.gov/em52/55105.html

Description Provided by Investigator:

The anaerobic treatment of short chain chlorinated aliphatics is a promising approach for remediating contaminated sites. The dehalogenation of 1,2-dichloropropane (1,2-DCP) under anaerobic conditions has not yet been explored and the sequential reductive dechlorination of tetra chloroethyene (PCE) is often incomplete and a substantial buildup of vinyl chloride (VC) is observed. Our approach to overcome these problems is based on the observation that chlororespiring organisms are involved in all of these dechlorination steps. Since these organisms benefit from the presence of the chlorinated compound, specific dehalogenating enzymes must be involved. We have obtained several highly enriched cultures dehalogenating chlorinated ethenes and 1,2-DCP from freshwater river sediments. *The research is focused on the isolation and characterization of pure cultures of halorespiring organisms that dechlorinate cis-DCE and VC to ETH and 1,2-DCP to propane, and on the purification and characterization of the dehalogenases responsible for these steps.* Understanding the physiology and phylogeny of these organisms and the biochemistry of the dehalogenating enzyme systems will greatly enhance our knowledge of how these organisms can be employed for successful bioremediation strategies.

Background and Significance

Short chain chlorinated aliphatics have been extensively used during the past decades due to their unique features, e.g., good solvent properties, easy availability, low cost, greatly reduced risk to fire and explosion and biocidal properties. Many of them have been widely employed as degreasing solvents, fumigants, dry-cleaning fluids as well as numerous other applications for industrial and domestic purposes. Furthermore, while some are intermediates in chemical synthesis, others are formed as undesired by-products. For example, 1,2-DCP is unintentionally produced in the chemical synthesis of propylene oxide using the chlorohydrin process. In 1991, 1.8×10^6 tons of propylene oxide were produced in the USA. Forty-two percent of this capacity was based on the chlorohydrin process with the concomitant formation of 6 to 9 % of 1,2-DCP. 1,2-DCP also has a wide application as a fumigant.

The widespread use along with careless handling, storage and disposal has made halogenated short chain aliphatics major environmental pollutants. Due to their relative high solubility in water, contamination of ground water and drinking water have been observed. Toxicological studies document the danger of halogenated short chain aliphatics. Many of them are known or suspected mutagens or carcinogens. Therefore the presence of halogenated short chain aliphatics in the environment is of public concern.

Tetrachloroethylene (PCE) and trichloroethylene (TCE) are among the most frequently detected ground water contaminants. Figure 1 shows the observed intermediates in the complete reductive dechlorination of PCE to ETH.

In laboratory studies with anaerobic microcosms, the subsequent reductive dehalogenation of PCE to TCE, dichloroethenes (DCE's), vinyl chloride (VC), ethene (ETH) and ethane has been observed. *cis*-DCE is the main intermediate in reductive PCE dechlorination and *trans*-DCE is only found, if at all, in small amounts. ETH and ethane are considered environmentally acceptable products. However, in many cases VC, a potent carcinogen, accumulated and the conversion to ETH was slow and incomplete. Today, the stepwise reductive dechlorination is problematic for the biological treatment of contaminated sites because of substantial VC accumulation. Thus, the main goal of this research is to gain more knowledge about organisms with the capability of completely detoxifying chlorinated ethenes.

In addition to chlorinated ethenes, chlorinated propanes are another group of permanent ground water pollutants. 1,2-DCP concentrations of 9 mg m^{-3} in ground water samples have been reported. In addition to their toxicity, with lung, reproductive organs, liver and kidney as the main target organs, chlorinated propanes were shown to be mutagenic and carcinogenic. However, we are not aware of any prior investigations on whether 1,2-DCP can be dechlorinated under anaerobic conditions. Use of this substrate also provides the potential for comparison of chloroalkane and chloroolefin dehalogenating systems.

Our approach to overcome this problem is based on the observation that chlororespiring organisms are involved in all of these dechlorination steps. Since these organisms benefit by enhanced energy and growth from the presence of the chlorinated compound, specific dehalogenating enzymes must be involved. This is an important distinction from organisms which co-metabolize some chlorinated aliphatics without the use of specific dehalogenating enzymes. Understanding the physiology and phylogeny of these chlororespiring organisms, and elucidating their dehalo genases, will greatly enhance our knowledge of how these organisms can be employed in successful bioremediation.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

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Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§ RL-ER08	C-147	Groundwater Management
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Michigan

University of Michigan

54548-MI - The Efficacy of Oxidative Coupling for Promoting In-Situ Immobilization of Hydroxylated Aromatics in Contaminated Soil and Sediment Systems

Year of Award: 1996 **Amount of Award:** $556,930
Problem Area: Remedial Action
Science Category/SubCategory: Geochemistry / Sorption/Desorption
Principal Investigator: Dr. Walter J. Weber, 313-763-2274, wjwjr@engin.umich.edu
For More Information: http://www.doe.gov/em52/54548.html

Description Provided by Investigator:

Hydroxylated aromatic compounds constitute an important class of commonly found subsurface organic contaminants. They have been classified as priority pollutants because of their multiple toxic health effects at very low concentrations. These compounds can be produced naturally or accumulate as intermediates during incomplete aerobic biodegradation of aromatic compounds and polycyclic aromatic hydrocarbons. Hydroxylated aromatics are listed among the 25 most frequently detected ground water contaminants at hazardous waste sites. These compounds and their precursors are commonly found in soils, sediments and groundwaters at DOE facilities nationwide.

Sorption is often the dominant process governing fate and transport of hydrophobic organic compounds in subsurface environments. Significant attention and extensive research efforts have been focused on the elucidation of fundamental mechanisms of sorption and desorption in various natural and model sorbent/sorbate systems. Chemical reactions between organic contaminants and soil/sediment organic and inorganic components have not been investigated extensively. Increasing evidence in the literature suggests that these chemical reactions, most specifically abiotic and/or enzymatic oxidative coupling, may be significant in controlling the fate of hydroxylated aromatics in subsurface systems. An important and even desirable consequence of abiotic or enzymatic coupling reactions is the immobilization of mono-and polycyclic hydroxylated aromatic compounds by irreversible binding to soil inorganic or organic matrices. Given sufficient knowledge regarding mechanisms, it may be plausible to induce such reactions in order to immobilize these common soil and groundwater contaminants *in-situ*, prevent environmental risks from their subsurface migration, and ultimately reduce costs of pump and treat systems.

The principal objectives of this study are to investigate: 1) the efficacy of abiotic/enzymatic coupling reactions on the irreversible binding of hydroxylated aromatic compounds on natural soil/sediment surfaces; 2) the contribution of abiotic and enzyme mediated coupling reactions to overall contaminant immobilization; 3) the role of environmental factors (e.g., pH, presence and absence of cofactors and oxidizing agents, soil organic and inorganic matrices) on abiotic/enzymatic coupling reactions in natural subsurface systems; 4) abiotic and enzymatic coupling reactions in model systems to get a basic understanding of the possible mechanisms for coupling reactions occurring in natural soils and sediments; and 5) preliminary engineering approaches for immobilization of hydroxylated aromatics in subsurface systems *in-situ.*

Three hypotheses have been raised to study these objectives. **Hypothesis 1)** Oxidative coupling reactions can be induced in contaminated subsurface systems to immobilize hydroxylated aromatic compounds on soil organic and inorganic matrices. **Hypothesis 2)** A basic understanding of the immobilization of hydroxylated aromatics and the conditions for their induction and control in contaminated subsurface environments can be obtained by a systematic investigation of abiotic and enzymatic coupling reactions in well defined model systems. The most critical system characteristics to investigate are: a) the soil organic matrices, b) the soilinorganic matrices, c) the chemical structure of the hydroxylated aromatic involved, and d) the composition of the background water. **Hypothesis 3)** Engineering approaches for immobilization of hydroxylated aromatic compounds in contaminated subsurface systems can be developed using the basic understanding obtained from natural and model system studies.

The above hypotheses will be tested experimentally using phenol, and methyl- and chlorosubstituted phenols and •-naphthol as model hydroxylated aromatic contaminants. Two different types of experimental systems will be investigated; one employing natural soil and sediment materials, and the other using well characterized model solids. The results obtained from investigations with natural soils and sediments will be correlated with: 1) the appropriate characteristics of these materials; 2) the types of hydroxylated aromatic compounds studied; and, 3) background environmental conditions. These correlations will put the experimental data into an application context. Results obtained from well defined and controlled model systems will be used to obtain mechanistic information regarding the oxidative coupling reactions, which in turn will be used to interpret the observations and findings from the natural system experiments.

Our understanding of the nature and extent of oxidative coupling reactions of hydroxylated aromatic compounds on soil and sediment surfaces should be markedly enhanced by this study. This in turn will facilitate assessment of the degree of reversibility of sorption of such compounds in subsurface systems, and thus their mobility and bioavailability. Coupling of such contaminants is expected to result in increased immobilization, with consequent reduction of risks posed to the environment. Information gathered from this study will be useful in quantifying subsurface contamination scenarios and strategies in the selection and design of remediation technologies.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

Environmental Management Science Program Research in Michigan

University of Michigan

54680-MI - The Migration and Entrapment of DNAPLs in Physically and Chemically Heterogeneous Porous Media

Year of Award: 1996 **Amount of Award:** $582,378
Problem Area: Remedial Action
Science Category/SubCategory: Hydrogeology / Dense Non-Aqueous Phase Liquid (DNAPL) Dynamics
Principal Investigator: Dr. Linda M. Abriola, 313-763-1464, abriola@engin.umich.edu
For More Information: http://www.doe.gov/em52/54680.html

Description Provided by Investigator:

Hazardous dense nonaqueous phase liquids (DNAPLs), such as chlorinated solvents, are slightly water soluble and pose a serious threat to soil and groundwater supplies in many portions of the United States. The migration and entrapment of DNAPLs in the subsurface environment is typically believed to be controlled by physical heterogeneities; i.e, layers and lenses of contrasting soil texture. The rationale for this assumption is that capillarity, as determined by the soil texture, is the dominant transport mechanism. Capillarity also depends on interfacial tension and medium wettability. Interfacial tension and medium wettability may be spatially and temporally dependent due to variations in aqueous phase chemistry, contaminant aging, and/or variations in mineralogy and organic matter distributions. Such chemical heterogeneities have largely been ignored to date, even though they are known to have dramatic effects on the hydraulic property relations. Numerical multiphase flow and transport models typically assume that solids are water-wet and that interfacial tension is constant. The primary objective of this research is to investigate the influence of coupled physical and chemical heterogeneities on the migration and entrapment of DNAPLs. This objective will be accomplished through a combination of laboratory and numerical experiments. Laboratory experiments will be conducted to examine: (i) aqueous phase chemistry effects on medium wettability and interfacial tension; and (ii) relative permeability-saturation-capillary pressure relations for chemically heterogeneous systems. An important objective of this research is to modify a two-dimensional multiphase flow and transport model to account for chemically and physically heterogeneous systems. This numerical simulator will be used in conjunction with independently measured parameters to simulate two-dimensional DNAPL infiltration experiments. Comparisons of simulated and laboratory data will provide a means to experimentally validate this model. The validated numerical simulator will subsequently be employed to investigate various innovative remediation schemes such as the use of surfactants and in situ wettability alteration. The accomplishment of the research herein will: (i) lead to a better understanding of the way aqueous phase chemistry changes medium wettability; (ii) validate and/or lead to the development of methods to predict and model wettability effects on hydraulic property relations; (iii) lead to the development of a multiphase flow simulator that accounts for fractional wettability and concentration dependent interfacial properties; (iv) lead to an improved knowledge of the effects of pore-scale variability on scale-up issues in multiphase systems; (v) provide an understanding of the interaction of chemical and physical heterogeneity on DNAPL flow and entrapment; (vi) provide two-dimensional laboratory data sets to validate multiphase flow models for physically and chemically heterogeneous systems; and (vii) facilitate the development and implementation of innovative remediation strategies.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ OR-46301	C-107	Portsmouth Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Michigan

University of Michigan

54691-MI - Radiation Effects on Materials in the Near-Field of Nuclear Waste Repository

Year of Award: 1996 **Amount of Award:** $408,000
Problem Area: High Level Waste
Science Category/SubCategory: Materials Science / Radiation Effects On Storage Materials
Principal Investigator: Dr. Lu-Min Wang, 313-647-8530, lmwang@umich.edu
Major Collaborator(s): Dr. Rodney C. Ewing at the University of Michigan
For More Information: http://www.doe.gov/em52/54691.html

Description Provided by Investigator:

Successful, demonstrated containment of radionuclides in the near-field can greatly reduce the complexity of the performance assessment analysis of a geologic repository. The chemical durability of the waste form, the corrosion rate of the canister, and the physical and chemical integrity of the back-fill provide important barriers to the release of radionuclides. However, near-field containment of radionuclides depends critically on the behavior of these materials in a radiation field.

The principal sources of radiation in high-level nuclear waste are β-decay of the fission products (e.g., ^{137}Cs and ^{90}Sr) and α-decay of the actinide elements (e.g., U, Np, Pu, Am and Cm). Both types of radiation can cause important chemical and physical changes in materials (e.g., increase in leach rates, volume expansion, solid state radiolysis and bubble formation, and reduced cation exchange capacity). The radiation-solid interactions are complex because they involve a combination of ionization effects due to electronic excitations and ballistic effects due to elastic collisions. The strength of the radiation field decreases dramatically with time, and the type of radiation damage varies over time (α-decay damage due to actinides dominates over β-decay effects due to fission products with increasing time due to the long half-lives of the actinides). Further, the radiation effects vary as a function of the type of solid (ionic *vs.* covalent), the type of damage (inelastic *vs.* elastic interactions), the temperature of the irradiation, and the kinetics of the annealing mechanisms.

We propose a systematic study of elastic and inelastic damage effects in materials in the near-field. These include: 1.) waste forms (glass and crystalline ceramics); 2.) alteration products of waste forms (clays and zeolites); 3.) back-fill materials (clays and zeolites). We have selected materials whose durability or chemical behavior can potentially have a major effect on the retention of radionuclides (e.g., monazite as a waste form; smectite clays in back-fill), *but* for which there is very little previous systematic study. We have not included canister materials in this research, as there is already a substantial body of previous work on radiation effects in metals.

The work draws on over twenty years of experience in studying radiation effects in minerals and complex ceramics and utilizes an unusual combination of studies of natural phases of great age with ion beam and electron irradiations of synthetic phases under carefully controlled conditions.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§ ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ RL-TW08	C-185	Process Waste Privatization Infrastructure
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
§ SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Michigan

University of Michigan

59849-MI - Radionuclide Immobilization in the Phases Formed by Corrosion of Spent Nuclear Fuel: The Long-Term Assessment

Year of Award: 1997 **Amount of Award:** $480,963
Problem Area: Spent Nuclear Fuel
Science Category/SubCategory: Geochemistry / Solid/Solution Geochemistry
Principal Investigator: Dr. Rodney C. Ewing, 313-647-8529, rewing@unm.edu
For More Information: http://www.doe.gov/em52/59849.html

Description Provided by Investigator:

The UO_2 in spent nuclear fuel is not stable under oxidizing conditions. Under oxic conditions, the U(IV) has a strong tendency to exist as U(VI) in the uranyl molecule, UO_2^{2+}. The uranyl ions react with a wide variety of inorganic and organic anions to form complexes which are often highly soluble. The result is rather rapid dissolution of UO_2 and the formation of a wide variety of uranyl oxide hydrates, uranyl silicates and uranyl phosphates. The reaction rates for this transformation are rapid, essentially instantaneous on geologic time scales. Over the long term, and depending on the extend to which these phases can incorporate fission products and actinides, these alteration phases become the near-field source term.

Fortunately, previous investigations (experimental studies and field studies) have established that natural uraninites and their alteration products can be used as *natural analogues* to study the corrosion of UO_2 in spent nuclear fuel. We propose in this research program to address the following issues:

1. What are the long-term corrosion products of natural UO_2+x, uraninite, under oxidizing conditions?

2. What is the paragenesis or the reaction path of the phases that form during alteration? How is the paragenetic sequence formation related to the structures and compositions of these uranyl phases?

3. What is the trace element content (as compared to the original UO_2+x), and does the trace element content substantiate models developed to predict fission product and actinide incorporation into these phases?

4. Are these the phases that are predicted from reaction path models (e.g., EQ3/6) which will be used in performance assessments?

5. How persistent over time are the metastable phase assemblages that form? Will these phases serve as barriers to radionuclide release?

6. Based on the structures of these phases (mostly sheet structures) can the thermodynamic stabilities of these phases be estimated, or at least bounded, in such a way as to provide for a convincing and substantive performance assessment?

This research is based on over a decade of previous work on uranium mineralogy, paragenesis, and the corrosion of UO_2 by the principal investigator, R. C. Ewing.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Spent Nuclear Fuel problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Spent Nuclear Fuel".

Environmental Management Science Program Research in Mississippi

Mississippi State University

60070-MS - The Development of Cavity Ringdown Spectroscopy as a Sensitive Continuous Emission Monitor for Metals

Year of Award: 1997 **Amount of Award:** $538,000
Problem Area: Mixed Waste
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Sensors and Techniques
Principal Investigator: Dr. George P. Miller, 601-325-7631, miller@dial.msstate.edu
For More Information: http://www.doe.gov/em52/60070.html

Description Provided by Investigator:

We propose to conduct an innovative science-driven technology program to explore the viability of using Cavity Ringdown Spectroscopy (CRS) to monitor the remediation processes for hazardous and radioactive wastes. This is a technique capable of providing ultra-sensitive absorption measurements ($<10^{-6}$ fractional absorption) in hostile environments using commercially-available easy-to-use pulsed lasers. This project has three primary goals: 1) Determine the viability, through experiment and model validation, of marrying an exciting new science tool - Cavity Ringdown Spectroscopy - with standard analytical instruments, e.g. the ICP and graphite furnace. 2) Provide the first ever quantitative evaluation of cavity ringdown spectroscopy for trace analysis. 3) Make a significant and positive impact in support of the management and disposal of DOE radioactive, hazardous chemical, and mixed waste. To accomplish these goals we have assembled a small, experienced, and highly motivated team of scientists who are committed to succeed.

Cavity ringdown spectroscopy (CRS) is a measurement of the rate of absorption of a sample within a closed optical cavity rather than the standard measurement of the absorbed signal strength over a given sample path. The inherent high sensitivity stems from both the long effective sample pathlengths possible (in the tens of kilometers) and the relaxed constraints on the accuracy of the measurement of the cavity decay time (-1% accuracy yields ppm absorbance detection capability).

Advantages of CRS for Atomic Absorption Spectrometry

1. Detection Limits attainable could exceed those achieved by ICP-MS.
2. Absorbance is linear with concentration. Increased dynamic range w.r.t AAS
3. Sensitivity increases as sample absorption decreases. Ideal for ultratrace measurement.
4. Reduced matrix effects compared to ICP-AES, AFS, or GF-AAS.
5. Potential high-sensitivity *on-line* offgas analysis (air-ICP-CRS) in environments hostile to MS.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§ ID-WM-107	C-45	Long Term Treatment/Storage/Disposal Operations
§ RL-WM03	C-193	Solid Waste Storage and Disposal
§ RL-WM04	C-197	Solid Waste Treatment
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW02	C-285	Transuranic Waste Project
§+ SR-SW03	C-287	Mixed Low Level Waste Project
ID-HLW-101	C-29	High-Level Waste Pretreatment
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-TW04	C-169	Retrieval Project
RF014	C-213	Industrial Zone Closure Project
+ SR-HL01	C-249	H-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Missouri

University of Missouri-Rolla

55110-MO - An Alternative Host Matrix Based on Iron Phosphate Glasses for the Vitrification of Specialized Nuclear Waste Forms

Year of Award: 1996 **Amount of Award:** $624,834
Problem Area: Mixed Waste
Science Category/SubCategory: Materials Science / Chemical and Structural Properties Of Storage Materials
Principal Investigator: Dr. Delbert E. Day, 573-341-4354, day@umr.edu
For More Information: http://www.doe.gov/em52/55110.html

Description Provided by Investigator:

Borosilicate glass is the only material currently approved and being used to vitrify high level nuclear waste. Unfortunately, many high level nuclear waste feeds in the U.S. contain components which are chemically incompatible with borosilicate glasses. Current plans call for vitrifying even these problematic waste feeds in borosilicate glasses after the original waste feed has been pre-processed and/or diluted to compensate for the incompatibility. However, these pre-treatment processes, as well as the larger waste volumes resulting from dilution. will add billions of dollars to the DOE's cost of cleaning up the former nuclear weapons production facilities. Such additional costs may be avoided by developing a small number of alternative waste glasses which are suitable for vitrifying those specific waste feeds that are incompatible with borosilicate glasses.

We have recently developed an alternative waste form based on a new family of iron-phosphate glasses which appear to be well suited for many waste feeds, especially those which are incompatible with borosilicate glasses. This previous work at the University of Missouri-Rolla, done in collaboration with scientists from *Pacific Northwest National Laboratory, Westinghouse Savannah River Laboratory, and Lawrence Berkeley National Laboratory*, strongly suggests that iron phosphate glasses are a low cost and highly, effective alternative to borosilicate glasses for vitrifying selected nuclear wastes.

More information on the atomic structure, valence states, nature of bonding, structure-property relationships, crystallization kinetics, and optimized melt processing conditions, is needed for iron phosphate glasses and their waste forms. In the research proposed herein, we intend to use techniques such as EXAFS, XANES, XPS, x-ray and neutron diffraction, IR, SEM, MÖssbauer spectroscopy and DTA/DSC to obtain the information needed to demonstrate that iron phosphate waste forms can meet the stringent requirements for nuclear waste disposal.

The overall objective of this work is to gain an understanding of those structure-property relationships for iron phosphate glasses that are of critical importance to cost-effective nuclear waste disposal. This research consists of a combination of structural modeling and analysis along with property measurements that will yield the informational data base of those property values and processing conditions directly applicable to nuclear waste disposal technology.

EXECUTIVE SUMMARY

In response to RFA. 96-10 issued by the office of Energy Research and Environmental Management of DOE, support is requested for a three year investigation on the atomic structure and properties of novel iron phosphate glasses. A basic premise of this research is that no single glass will be a cost-effective means of vitrifying all of the widely different nuclear wastes that have been identified at various DOE sites and that a small number of alternative waste glasses will be needed.

Preliminary studies at the University of Missouri-Rolla, in cooperation with the Pacific Northwest Laboratories and Westinghouse Savannah River Laboratory, show that iron phosphate glasses have the potential for vitrifying many radioactive wastes which are not well suited for borosilicate glasses. Iron phosphate glasses are considered a viable alternative for vitrifying those wastes at several DOE sites, which are high in phosphates, iron oxides, and heavy metals. Information on the structure and properties of these glasses is presently limited but such information is essential to assess the properties and long term performance of iron phosphate wastes.

The research on the iron phosphate glasses will focus on four areas, namely, (1) investigating the glass composition and processing conditions that yield optimum properties for vitrifying radioactive waste, (2) determining the atomic structure of these glasses and how it influences selected properties, (3) determining how the physical and structural properties are affected by the addition of simulated radioactive waste components, and (4) investigating the process and products of devitrification of the waste forms.

Iron phosphate glasses, both of varying composition and containing simulated nuclear waste components, will be synthesized under controlled processing conditions (atmosphere/temperature/time). The density, thermal expansion, softening, crystallization and liquids temperatures will be measured for each glass. The chemical durability and its dependence on the composition, processing condition, and pH of the test solutions will be investigated for iron phosphate glasses and their crystalline counterparts. The long and short range structure, coordination number, and chemical bonding of the atomic/ionic species will be studied using Mössbauer, photoelectron, and infrared spectroscopies, x-ray and neutron diffraction, and extended x-ray absorption fine structure analysis. Selected glasses will be thermally crystallized and the products of crystallization will be analyzed by x-ray and neutron diffraction and electron microscopy. The process and kinetics of crystallization will be investigated by differential thermal analysis.

At the conclusion of this work, the DOE will have an information base for iron phosphate glass waste forms that should provide a cost effective alternative to using borosilicate glass waste forms. The properties of selected iron phosphate glass waste such as their chemical durability will be known, the important processing variables (melting time/temperature/ atmosphere) will have been identified and optimized, and their property-structure relationships will be understood. These results should be sufficient for the DOE to undertake an economic and technical assessment of iron phosphate glass waste forms.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

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Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§+ SR-SW03	C-287	Mixed Low Level Waste Project
ID-HLW-101	C-29	High-Level Waste Pretreatment
ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
+ RL-TW05	C-173	Process Waste Support
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
+ RL-TW08	C-185	Process Waste Privatization Infrastructure
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
+ SR-HL01	C-249	H-Tank Farm
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Missouri

Washington University

55223-MO - De Novo Design of Ligands for Metal Separation

Year of Award: 1996 **Amount of Award:** $380,000
Problem Area: Mixed Waste
Science Category/SubCategory: Separations Chemistry / Ligand Design and Ion-exchange
Principal Investigator: Dr. Garland R. Marshall, 314-361-1567, GARLAND@WUCMD.WUSTL.EDU
For More Information: http://www.doe.gov/em52/55223.html

Description Provided by Investigator:

This application focuses on the development of appropriate computation tools and parameters for the de novo design of selective metal ligands. We have developed a successful suite of tools for computer-aided design of ligands for receptors of known three-dimensional structure (structure-based design), including the prediction of affinity. Adaptation of the algorithms to place donor atoms at appropriate geometrical locations surrounding the metal of interest, rather than filling up a cavity with donor/acceptor atoms placed optimally to interact with a protein active site, is straightforward. Appropriate geometrical parameters for metals can be derived from crystal structures and force constants adapted from recent advances in theories of metal-ligand interactions. The practical goal is computer-aided design of ligands which would be selective for one metal over another with a predicted selectivity ratio and affinity.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW03	C-287	Mixed Low Level Waste Project
ID-HLW-101	C-29	High-Level Waste Pretreatment
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
+ RL-TW04	C-169	Retrieval Project
+ RL-TW05	C-173	Process Waste Support
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project
+ SR-HL01	C-249	H-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations

Environmental Management Science Program Research in New Hampshire

Dartmouth College

60271-NH - Characterization of a New Family of Metal Transport Proteins

Year of Award: 1997 **Amount of Award:** $600,000
Problem Area: Remedial Action
Science Category/SubCategory: Plant Science / Plant Membrane Transport
Principal Investigator: Mary Lou Guerinot, 603-646-2527, Guerinot@Dartmouth.edu
Major Collaborator(s): David Eide at the University of Missouri at Columbia
For More Information: http://www.doe.gov/em52/60271.html

Description Provided by Investigator:

Little is known about how plants take up heavy metals. Before plants can be engineered for use in phytoremediation strategies, basic information is needed on metal ion uptake and its regulation. Integrating genetic, molecular biological and biochemical approaches, we will examine these processes in the yeast *Saccharomyces cerevisiae* and the plant *Arabidopsis thaliana.* Both are proven model systems for studying fundamental cellular processes. Indeed, at this time, the only known eukaryotic genes that encode metal uptake transporters have been isolated from these two organisms. We have recently identified a new group of eukaryotic metal transporters namee the ZRT-, IRT-like Protein or ZIP gene family. This name is derived from the first members to be studied, the *ZRT1.* and *ZRT2* genes of *S. cerevisiae* and the *IRT1* gene of *Arabidopsis.* In addition to these genes, we have identified six ZIPs in plants, four in nematodes and two in humans. Our published and preliminary studies demonstrate that ZIP proteins are metal transporters. *IRT1* encodes an FE(II) transporter whereas *ZRT1*, *ZRT2* and three genes from *Arabidopsis* (ZIP1, ZIP2, ZIP3) encode Zn(II) transporters. It is a central hypothesis of our research that ZIP genes play pivotal roles in metal ion transport in most, if not all, eukaryotes. Thus, study of the ZIP gene family gives us a unique opportunity to achieve two goals of vital interest to DOE: 1) To clean up sites contaminated with heavy metals using our knowledge to design plants that can readily take up metals from such sites and 2) To assess how readily metals move through the food chain using our knowledge of the biochemical principles that govern metal uptake. In the course of our studies, we have identified an important feedback system, called feedback inactivation, that prevents metal overaccumulation and toxicity. In yeast, ZN(II) causes a dramatic increase in the rate of degradation of the *ZRT1* protein. In *Arabidopsis*, transgenic plants that overexpress the *IRT1* transporter at the mRNA level do not accumulate *IRT1* protein unless the plant is iron-deficient, paralleling the results we see in yeast. Thus, it is clear from our preliminary studies that targeted overexpression of a plasma membrane transporter is not sufficient to confer dominant, gain-of-function enhancement of metal uptake. We are proposing to 1) determine the role of ZIP transporters in *Arabidopsis* metal ion uptake and metabolism, 2) identify residues that determine substrate affinity and specificity and 3) characterize the post-translation feedback inactivation mechanism in ZIP transporters. With knowledge gained from our studies, we will then 4) design transgenic plants that are able to accumulate specific heavy metals. Ultimately, our research will lead to a better understanding of metal ion uptake and homeostasis in humans. Such an understanding is essential for assessing the risk to human health from exposure to ingested metals, as regulatory systems like feedback inactivation may help limit uptake of metal ions from the diet.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV212	C-49	Underground Test Area (UGTA)
§ NV214	C-53	Industrial Sites
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER02	C-129	200 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation

Environmental Management Science Program Research in New Jersey

University of Medicine and Dentistry of New Jersey

54584-NJ - Comparison of the Bioavailability of Elemental Waste Laden Soils Using in vivo and in vitro Analytical Methodology, and Refinement of Exposure/Dose Models

Year of Award: 1996 **Amount of Award:** $506,040
Problem Area: Health / Ecology / Risk
Science Category/SubCategory: Health Science / Biophysics/Dose
Principal Investigator: Dr. Paul J. Lioy, 908-445-0155, plioy@eohsi.rutgers.edu
For More Information: http://www.doe.gov/em52/54584.html

Description Provided by Investigator:

Hazardous waste contamination problems are prevalent in soils at DOE sites. Currently, they can be prioritized by estimating the human exposure and health risks from potential human contact with contaminants based upon the total extractable levels of contaminants of concern present in the soil or soil/waste matrix. This is done for single and multi-route exposure conditions with exposure via ingestion of contaminants in the soil being a major concern. Since it is anticipated that portions of some DOE sites will have parkland, commercial or residential restorations, a major concern is exposure of children to wastes. Studies have shown that children ingest between 40-200 mg of soil/day, and that children who suffer from PICA will ingest even larger quantities. These data have been tabulated by the American Industrial Research Council. The total extractable concentration of a contaminant present in the soil is not the best estimator of exposure since the human digestive system does not have the capacity to extract all of the contaminant from a soil matrix. Conversely, a determination of the bioavailable portion of the contaminants in the soil/waste can be used by risk analysts and assessors to more accurately estimate the risk via ingestion for individual waste sites. Use of the concentration present in a simulated bioavailable fraction is a better indicator of ingestion risk from a waste contaminated soil because it represents the portion of the contaminant mass which will yield exposure, uptake and then the internal dose to an individual or a sub-group of a population. To date the difficulty in obtaining an accurate assessment of the internal dose is caused by the lack of scientific information on the degree to which a contaminant will accumulate in bodily fluids and will be made available for migration across the membranes within the digestive system. The uncertainties associated with exposure/dose calculations derived from total elemental concentrations can be overcome by developing a procedure that accurately estimates the bioavailable fraction of the contaminant found in a particular soil or soil/waste mixture. Some previous research has been conducted which examined the possibility of developing a synthetic extraction fluid system. A physiologically based bioaccessibility test for lead and arsenic has been published by Ruby et al. for mining crustal material. They have also evaluated geochemical and physiological variables, and made comparisons with *in vivo* rabbit data and dissolution kinetics of the crustal material under simulated gastric conditions. The TNO Nutrition and Food Research Institute of the Netherlands focuses on the bioavailability of inorganic arsenic from Bog-ore. They use a system to mimic the stomach and intestine. Our system is the only one to use all digestive juices, and attempts to look at a variety of different types of waste-soil situations. It will be used as the basis for the experiments.

Previous research conducted by our laboratory on waste-laden soils in New Jersey, has shown that in specific situations, e.g. sites contaminated with dioxin and chromium, the matrix that binds a toxicant to the soil or components within the soil will alter the availability of the contaminants to be solvated by different extractants. If it is difficult to liberate the total concentration of the elements from a soil, even with concentrated acids and high temperatures and pressures, then the bioavailability of the elements would be uncertain. The bioavailability of elemental contaminants should be estimated by extracting with biological fluids (e.g. intestinal fluids). Analysts have routinely relied on a conventional definition of total extractable elements obtained by using EPA method 3015, 3050, or 3051 when reporting a soil concentration used in an exposure assessment. In reality, bio-fluids may only solubilize a small percentage of the totalelements present in the soil, and traditional extraction techniques can lead to artificially high estimates of internal dose, and uncertain/unrealistic estimates of the risk to a population.

The extractability of contaminants affects its transport into various organ systems within the body. Assuming the contaminants will undergo dissolution and absorption by specific target tissues and organs, artificially high estimations of the bioavailable fraction or 100% bioavailability will alter internal dose estimates. The ratio of the total amount of material present in the soil/waste matrix to that which is available for dissolution in a bio-fluid extractant gives an indication of the bioavailability of the contaminant.

Our hypotheses are: 1) the more closely the synthetic, *in vitro*, extractant mimics the extraction properties of the human digestive bio-fluids, the more accurate will be the estimate of an internal dose; 2) performance can be evaluated by *in vivo* studies with a rat model and quantitative examination of a mass balance calculation, and dose estimates from model simulations for the *in vitro* and *in vivo* system; and 3) the concentration of the elements Pv, U, Cd, Cr and Cs present in the bioavailable fraction obtained with a synthetic extraction system will be a better indicator of contaminant ingestion from a contaminated soil because it represents the portion of the mass which can yield exposure, uptake and then the internal dose to an individual.

Rationale

Our concern about bioavailability is derived from the fact that a major route of exposure to elements present in soils and hazardous wastes is through ingestion, especially among young children. For example, soil accumulates on the hand, or in food, and it is then transferred to the mouth by normal activities: consuming food, wiping one's mouth, or teething, etc. Once inside the mouth the soil will encounter the same biological processes that are encountered by edible material. It will interact in succession with saliva, gastric juice and the intestinal fluids under physiological conditions of temperature and pH. It is under this sequence of conditions that the data derived from a synthetic bio-fluid extraction system can provide a more accurate assessment of the potential or internal doses for elements.

Previous research with synthetic bio-fluids has been directed toward different aspects of physiological modeling. Synthetic analogs have been used to predict uptake of drugs, or nutritional compounds from food supplements. They have been used to model wear characteristics of watches or tooth fillings. They have also been employed at EOHSI and in other laboratories to begin to define the bio-available fraction of a contaminated matrix. Although each study has had different goals and the synthetic bio-fluids were prepared with different degrees of thoroughness, they all showed that the bio-fluids could not extract the target compound from a matrix with 100% efficiency. Recently Ruby et al. looked at the bioavailability of arsenic in a specific matrix, mining crustal material, and showed significant amounts as being unavailable for extraction. The developmental studies currently underway in the EOHSI laboratories are performed in a sequential synthetic digestive extraction system which was reacted with NIST Montana soil. The extraction efficiency was found to be 50% or less for the metals: Cd, As, and Pb and roughly 5% for Cr. The synthetic system was then applied to an actual soil/waste site mixture from Jersey City, NJ. The results found that only 4% of the chromium, and 3% of the lead extracted by concentrated acid digesting at a high temperature could be extracted by the EOHSI synthetic bio-fluids system. This system most closely follows the physiological digestion process, and will be used as the basic extraction system for the experiments.

Elemental solubility in a bio-fluid is expected to be dependent on both the soil matrix and the form of the metal within the soil. The variety of soil and crustal material present in urban locations throughout the United States complicates the situation since a potential exposure should be characterized using the site specific analyses. Unfortunately, this is not currently the case. The degree to which elements bind to a matrix may be also governed by some of the same thermodynamic properties that govern its transport properties through the soil.

With the number of DOE hazardous waste sites in the United States that require risk assessment, use of animal models as the main vehicle for determining the bioavailable fraction is neither practical nor cost effective. A general technique to extract soils or wastes that employs synthetic bio-fluids that approach physiological conditions can be a practical cost effective alternative to animal studies and it can be done routinely on a wide variety of soil and soil/waste mixtures. It can also be tailored to more closely match the concentrations of physiological constituents found in a human. The research will be able to evaluate the performance of a synthetic bio-fluid extraction system using an *in vivo* animal model as the reference for bioavailability of each element.

Specific Aims of Project

1.Use the synthetic analogs in a model system to extract elements from actual waste laden soils before and after application of remediation strategies and determine the bioavailable fraction of those elements under typical physiological conditions.

2.Conduct a performance experiment for selected known wastes using an *in vivo* animal (rat) feeding model and the synthetic analog digestive system model to compare the percentage of each element that is bioavailable in each model.

3.Conduct exposure analyses and dose analyses using the elements extracted by each "ingestion" experiment conducted in #3 and for the total elemental concentrations extracted from the soil/waste matrix and compare the results.

4.Improve our current exposure/pharmacokinetic components of the Exposure and Dose Modeling and Analysis System (EDMAS) for better estimations of the internal and delivered dose.

5.Optimize the synthetic extraction methodology employed for use as a routine assay of contaminated soils.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Health / Ecology / Risk problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Health / Ecology / Risk".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in New Mexico

Los Alamos National Laboratory

54724-NM - Synthesis of New Water-Soluble Metal-Binding Polymers: Combinatorial Chemistry Approach

Year of Award: 1996 **Amount of Award:** $1,120,000
Problem Area: Decontamination and Decommissioning
Science Category/SubCategory: Inorganic Chemistry / Solid/Solution Chemistry
Principal Investigator: Dr. Barbara F. Smith, 505-667-2391, bfsmith@lanl.gov
Major Collaborator(s): Dr. R. Bryan Miller at the University of California at Davis
Dr. Mark J. Kurth at the University of California at Davis
Dr. Samuel Sawan at the University of Massachusetts at Lowell
For More Information: http://www.doe.gov/em52/54724.html

Description Provided by Investigator:

A variety of metals that require removal and concentration exist in DOE waste, ground, or process waters. These can include, for example, RCRA metals such as mercury in mixed waste, valuable metals such as copper in acid mine drainage, actinides in plutonium processing facilities, and fission products such as technetium in groundwater or Hanford Tanks. A robust process, Polymer Filtration®, that can address the various conditions that these dilute waste streams present, is under development for aqueous stream polishing. Polymer Filtration® combines specially prepared water-soluble metal-binding polymers with commercially available ultrafiltration membranes to effect a selective separation of metal ions. To further the development of this technology the discovery and optimization of new, selective, strong, and reversible chelating polymers is necessary. To speed this process we are adapting an approach called combinatorial chemistry that is used in the pharmaceutical industry for drug discovery. This research will explore the combinatorial approach for the discovery of metal-binding chelators attached to water-soluble polymers.

To demonstrate the process, two target ligands will include the structure rich 1,3-dicarbonyl compounds encompassed in the acylpyrazolones and the 1,2-diols. These compounds were chosen because of the diversity of metals that they will target from tetravalent actinides to the oxyanions. The new materials will be assayed using a variety of techniques including radiolabeling and x-ray fluorescence spectroscopy. The new lead materials will then be prepared in larger quantity for further evaluation of their physical properties of stability, solubility, capacity, etc. and will be probed spectroscopically to identify the specific nature of their binding sites using NMR and other spectroscopic techniques. It is anticipated that new materials will be developed that will be able to address many DOE metal removal/recovery needs. These new materials are poised for transition to industry because of our current industrial partnerships.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Decontamination and Decommissioning problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Decontamination and Decommissioning".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
§ OR-43204	C-77	ORNL Bethel Valley Deactivation and Decommissioning
§ OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
§+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
§+ RL-ER06	C-141	Decontamination and Decommissioning
§+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
§ RL-TP10	C-163	Accelerated Deactivation
AL024	C-3	Grand Junction Office (GJO) All Other Projects
ID-HLW-101	C-29	High-Level Waste Pretreatment
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
+ OR-48101	C-99	Offsite Remedial Action
+ OR-45301	C-103	Paducah Remedial Action
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
RL-ER08	C-147	Groundwater Management
+ RL-TW05	C-173	Process Waste Support
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project
+ SR-HL01	C-249	H-Tank Farm
+ SR-HL02	C-253	F-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
SR-HL05	C-265	Vitrification
+ SR-SW01	C-281	Consolidated Incinerator Facility
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in New Mexico

Los Alamos National Laboratory

54741-NM - Characterization of Contaminant Transport Using Naturally-Occurring U-Series Disequilibria

Year of Award: 1996 **Amount of Award:** $900,295
Problem Area: Remedial Action
Science Category/SubCategory: Geochemistry / Sorption/Desorption
Principal Investigator: Dr. Michael Murrell, 505-667-4845, mmurrell@lanl.gov
Major Collaborator(s): Dr. Teh-Lung Ku at the University of Southern California
For More Information: http://www.doe.gov/em52/54741.html

Description Provided by Investigator:

The interactions of mixed wastes containing radionuclides with solid rock surface and the mobility of the radionuclides in aquifer systems depend not only on the chemistry of the nuclides and the physico-chemical effects of radioactive decay, but also on the site-specific hydrogeology. Thus, to characterize contaminant transport, it is best to cross-check figures derived from any small-scale laboratory experiments over limited times with that obtained from field-oriented, natural analog studies. We propose such a study using the naturally-occurring U and Th decay-series disequilibria. The work of ours and other researchers have shown that the parent/daughter disequilibrium patterns existing in groundwater systems can be modeled in terms of local nuclide mass balance to arrive at such information as the rock-water contact time (fluid flow) and rates of contaminant transport (taking into account the retardation effect due to nuclide/rock interaction contaminants at INEL by grouping them into three categories, represented by isotopes of (1) Th and Pa, (2) U and (3) Ra. Mass spectrometric measurements of these elements will be emphasized in order to minimize sample size requirements and to maximize precision. Results will form the data base for a model code for computing : (1) Fluid residence time (transport rates) in the basalt aquifers at various locations, (2) The in-situ adsorption and desorption rate constants, as well as the retardation factors, of various radionuclide wastes, and (3) Rock dissolution rate and its relation to preferential flow and contaminant transport in the fractured rocks.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ AL007	C-7	Environmental Restoration
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV212	C-49	Underground Test Area (UGTA)
§ NV214	C-53	Industrial Sites
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
SR-HL03	C-257	Waste Removal Operations and Tank Closure

Environmental Management Science Program Research in New Mexico

Los Alamos National Laboratory

54751-NM - High Fluence Neutron Source for Nondestructive Characterization of Nuclear Waste

Year of Award: 1996 **Amount of Award:** $745,139
Problem Area: Mixed Waste
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Sensors and Techniques
Principal Investigator: Dr. Mark M. Pickrell, 505-665-5098, pickrell@safeguard.lanl.gov
For More Information: http://www.doe.gov/em52/54751.html

Description Provided by Investigator:

We propose to research the basic plasma physics necessary to develop a high fluence neutron source based on the inertial electrostatically confined (IEC) plasma. An intense neutron source directly addresses the capability to characterize nuclear materials under difficult measurement conditions. Some of the applications for Environmental Management are the characterization of TRU wastes for WIPP (particularly remote handled [RH]), the measurements of residues prior to stabilization and disposal, the measurements of cemented or vitrified wastes, the measurement of spent nuclear fuel, and the measurement of high level wastes. Existing technology is insufficient to measure these contaminants because it addressed a substantially different technical problem: the measurement of very pure material. However, the present need is to develop measurement capability for highly impure, contaminated, and heterogeneous materials that are the wastes and residues of the production process. These measurement conditions demand measurement capabilities several orders of magnitude above existing capabilities. This neutron source could extend existing instrumentation sufficiently to meet these requirements. The benefit of this approach is that mature, neutron-based, nondestructive characterization methods could be used, but their capabilities would be increased by the same amount as the increase in neutron intensity. We propose to develop a source at the 10^{11} n/s level, with a cost, weight, and size comparable to 10^{8} n/s systems, for a 3 order of magnitude improvement.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§ ID-WM-107	C-45	Long Term Treatment/Storage/Disposal Operations
§ RL-WM03	C-193	Solid Waste Storage and Disposal
§ RL-WM04	C-197	Solid Waste Treatment
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW02	C-285	Transuranic Waste Project
§+ SR-SW03	C-287	Mixed Low Level Waste Project
AL024	C-3	Grand Junction Office (GJO) All Other Projects
AL007	C-7	Environmental Restoration
+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
ID-HLW-101	C-29	High-Level Waste Pretreatment
ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
NV212	C-49	Underground Test Area (UGTA)
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
+ OR-45301	C-103	Paducah Remedial Action
+ OR-46301	C-107	Portsmouth Remedial Action
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
RL-ER08	C-147	Groundwater Management
+ RL-TW05	C-173	Process Waste Support
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW08	C-185	Process Waste Privatization Infrastructure
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
+ SR-ER06	C-227	Upper Three Runs Project
+ SR-HL01	C-249	H-Tank Farm
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in New Mexico

Los Alamos National Laboratory

54765-NM - Enhanced Sludge Processing of HLW: Hydrothermal Oxidation of Chromium, Technetium, and Complexants by Nitrate

Year of Award: 1996 **Amount of Award:** $1,020,000
Problem Area: High Level Waste
Science Category/SubCategory: Inorganic Chemistry / Hydrothermal Oxidation
Principal Investigator: Dr. Steven J. Buelow, 505-667-1178, buelow@lanl.gov
For More Information: http://www.doe.gov/em52/54765.html

Description Provided by Investigator:

Efficient separation of chromium from high-level waste (HLW) sludge could save in excess of $3.4B for Hanford tank wastes. New chemical processes are needed to separate chromium and other metals from tank wastes. Our objective is to lay the foundation for the application of hydrothermal processing to high level wastes for enhanced chromium separation from sludges. We will determine the rates of oxidation and the products for the reactions of α-Cr_2O_3, mixed Fe:Cr species, and other selected minerals in simple hydrothermal solutions containing NaOH and $NaNO_3$. We will also examine the effects of additional components (EDTA, aluminate, carbonate, nitrite, phosphate, chloride, nickel, iron) on reaction chemistry. Studies will be conducted at temperatures and pressures ranging from 150 to 550°C and 10 to 1000 bar. The phase behavior and diffusion constants of selected species and mixtures will be determined. A reaction model will be formulated from experimental results and compared to experimental data for validation. The speciation of technetium and TRU will be examined in waste samples and waste simulants at hydrothermal conditions optimal for chromium dissolution.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§ ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations

Environmental Management Science Program Research in New Mexico

Los Alamos National Laboratory

54770-NM - New Anion-Exchange Resins for Improved Separations of Nuclear Materials

Year of Award: 1996 **Amount of Award:** $1,212,211
Problem Area: Mixed Waste
Science Category/SubCategory: Separations Chemistry / Ligand Design and Ion-exchange
Principal Investigator: Dr. Mary E. Barr, 505-667-7991, mbarr@lanl.gov
Major Collaborator(s): Dr. Richard A. Bartsch at Texas Tech University
For More Information: http://www.doe.gov/em52/54770.html

Description Provided by Investigator:

Improved separations of nuclear materials will have a significant impact upon a broad range of DOE activities. DOE-EM Focus Areas and Crosscutting Programs have identified improved methods for the extraction and recovery of radioactive metal ions from process, waste, and environmental waters as critical needs for the coming years. We propose to develop multifunctional anion-exchange resins that facilitate anion uptake by carefully controlling the structure of the anion receptor site. Our new ion-exchange resins interface the field of ion-specific chelating ligands with robust, commercial ion-exchange technology to provide materials which exhibit superior selectivity and kinetics of sorption and desorption. The following Focus Areas and Crosscutting Programs have described needs that would be favorably impacted by the new materials:

Efficient Separations and Processing - radionuclide removal from aqueous phases

Plutonium - Pu, Am or total alpha removal to meet regulatory requirements before discharge to the environment

Plumes - U and Tc in groundwater; U, Pu, Am, and Tc in soils

Mixed Waste - radionuclide partitioning

High-Level Tank Waste - actinide and Tc removal from supernatants and/or sludges

The basic scientific issues which need to be addressed are actinide complex speciation along with modeling of metal complex/functional site interactions in order to determine optimal binding-site characteristics. Synthesis of multifunctionalized extractants and ion-exchange materials that implement key features of the optimized binding site, and testing of these materials, will provide feedback to the modeling and design activities. Resin materials which actively facilitate the uptake of actinide complexes from solution should display both improved selectivity and kinetic properties. The long-range implications of this research, however, go far beyond the nuclear complex. This new methodology of 'facilitated uptake' could revolutionize ion-exchange technology, allowing this robust, inexpensive procedure to attain unprecedented levels of ion affinity and selectivity.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW03	C-287	Mixed Low Level Waste Project
ID-HLW-101	C-29	High-Level Waste Pretreatment
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW04	C-169	Retrieval Project
+ RL-TW05	C-173	Process Waste Support
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project
+ SR-HL01	C-249	H-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations

Environmental Management Science Program Research in New Mexico

Los Alamos National Laboratory

54773-NM - Microstructural Properties of High Level Waste Concentrates and Gels with Raman And Infrared Spectroscopies

Year of Award: 1996 **Amount of Award:** $465,000
Problem Area: High Level Waste
Science Category/SubCategory: Materials Science / Waste Materials
Principal Investigator: Dr. Stephen F. Agnew, 505-665-1764, sfagnew@lanl.gov
For More Information: http://www.doe.gov/em52/54773.html

Description Provided by Investigator:

Nearly half of the high level radioactive waste stored at Hanford is composed of highly alkaline concentrates referred to as either salt cakes or Double-Shell Slurry (DSS), depending on their compositions and processing histories. The major components of these concentrates are water, sodium hydroxide, and sodium salts of nitrate, nitrite, aluminate, carbonate, phosphate, and sulfate. In addition, there are varying amounts of assorted organic salts such as EDTA, glycolate, and citrate. Although measurements of the bulk properties of these wastes, such as viscosity, gel point, density, etc., have been exhaustively reported in the past, little is known about how those macroscopic characteristics are related to the microscopic physical and chemical properties of the waste. Such characteristics as viscosity, solids volume percent, and gas retention can change dramatically with relatively small changes in composition and temperature and these same properties are important for the determination of safe storage conditions as well as in planning retrieval, pretreatment, and disposal of the wastes.

The aim of this work is to use FTIR, Raman, and NMR spectroscopies along with thermophysical heats of gelation to relate the microstructural physical and chemical properties of these concentrates to their macroscopic characteristics. With this better understanding of macroscopic characteristics, the DOE will be in a better position to safely store these wastes as well as to be able to better plan for their retrieval, pretreatment, and final disposal. We will relate these microscopic properties to the macroscopic characteristics by using:

- Water vapor pressure measurements for concentrates to unambiguously determine water activity as a function of composition and temperature.

- FTIR, Raman, and Al NMR spectroscopies to determine the form and solubility of aluminate in caustic slurries. For example, is the aluminate dimer significantly less soluble than the monomer? What effects do competing ions and water activity have on aluminate dimerization?

- Micro-Raman spectroscopy to identify and quantify phases of each species for a variety of concentrates.

- Measurements of the heat of gelation and its dependence on water activity, presence of organic, and other properties.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ RL-TW04	C-169	Retrieval Project
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations

Environmental Management Science Program Research in New Mexico

Los Alamos National Laboratory

59967-NM - Aqueous Electrochemical Mechanisms in Actinide Residue Processing

Year of Award: 1997 **Amount of Award:** $750,000
Problem Area: Nuclear Materials
Science Category/SubCategory: Actinide Chemistry / Actinide (Heavy Element) Chemistry
Principal Investigator: Dr. David E. Morris, 505-665-6487, demorris@lanl.gov
Major Collaborator(s): Dr. David L. Blanchard Jr. at Pacific Northwest National Laboratory
For More Information: http://www.doe.gov/em52/59967.html

Description Provided by Investigator:

The United States Department of Energy is faced with the stabilization and disposition of hundreds of metric tons of plutonium - and uranium-bearing residue materials resulting from 50+ years of nuclear weapons production activities. These materials are presently in storage at sites throughout the weapons production complex, and they pose an immediate potential threat due to instability and degradation, and a long-term problem because the volume of material is to be disposed may exceed projected repository capacities. New and/or improved solutions to the stabilization and volume reduction of these residues are urgently needed. Mediated electrochemical oxidation/reduction (MEO/R) processes for dissolution of the actinide material from these residues are one such approach. They are low temperature, ambient pressure processes that operate in a non-corrosive environment, they can be designed to be highly selective for the actinides (i.e., no substrate degradation occurs), and they can be utilized for many categories of residue materials with little or no modification in hardware or operating conditions.. However, many fundamental questions remain concerning the mechanisms through which these processes act, and how the processes might be optimized to maximize efficiency while minimizing secondary waste. In addition, further research is merited to extend the range of applicability of these electrochemical methods to other residue and waste streams.

Recent advances in the study of heterogeneous electron transfer in transition-metal oxide and other semiconductor colloids have opened an exciting new door for the re-examination of the electron transfer processes associated with redox mediated actinide dissolution. We will take full advantage of this exciting new science to develop a new and deeper understanding of the thermodynamic and mechanisitic aspects of heterogeneous electron transfer that lie at the heart of these MEO/R processes. We will also develop and test new approaches based on the results of these fundamental studies using actual residue materials. Key aspects of this research include:

- Determination of the thermodynamic potential windows for oxidation/reduction of colloidal actinide oxides and actinide-bearing oxide and organic substrates and the associated electron-transfer kinetic parameters (including those for solid-phase diffusion processes) that govern the current - overpotential characteristics required to sustain redox mediated actinide dissolution without degradation or destruction of the residue substrate.

- Development and investigation of novel adaptations of electrochemical mediation schemes including studies of reductive dissolution processes (Pu(IV) to Pu(III) and application of co-mediation or co-catalysis reagents for both oxidative and reductive dissolution based on complexation of the surface-bound or solid-phase actinides and/or the dissolved redox mediator to manipulate the redox potentials, the solution-phase solubility, and the surface dissolution rates of the system components.

- Execution of bench-scale tests of new MEO/R schemes on actual residue materials in storage at Los Alamos and Pacific Northwest National Laboratory to assess rates and extents of actinide removal under conditions that simulate engineering process scale.

The work proposed here will revolutionize mediated electrochemical dissolution technology by providing selective, tunable schemes for actinide removal without degrading the residue substrate. These studies will progress in a sufficiently timely manner for consideration in meeting current stabilization deadlines (FY 2002), and they will contribute significantly to the ongoing effort directed at waste minimization/pollution prevention associated with continued actinide processing activities and waste-form and spent fuel stabilization assessment.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Nuclear Materials problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Nuclear Materials".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in New Mexico

Los Alamos National Laboratory

59981-NM - Real-Time Broad Spectrum Characterization of Hazardous Waste by Membrane Introduction Mass Spectrometry

Year of Award: 1997 **Amount of Award:** $655,000
Problem Area: Mixed Waste
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Mass Spectrometry
Principal Investigator: Dr. Philip H. Hemberger, 505-665-5735, hembergerph@lanl.gov
For More Information: http://www.doe.gov/em52/59981.html

Description Provided by Investigator:

We propose to expand the real-time monitoring capabilities of Membrane Introduction Mass Spectrometry (MIMS) to the pivotal problem of Mixed Hazardous Wastes, with secondary emphasis on monitoring incinerator stack gases for both organics and toxic metals. The methodologies developed in this research could also be applied to other environmental and effluent monitoring problems that require highly sensitive, on-line detection of a wide variety of chemicals including both volatile and semi-volatile organic compounds, and heavy metals.

Membrane introduction mass spectrometry is well-developed for the on-line analysis of volatile organic compounds (VOCs) in air and water. We propose the research and development necessary to develop a MIMS methodology for broad range characterization of both organic and heavy metal contaminants in a variety of matrices and effluents. In the MIMS experiment, a polymer membrane is the interface between the sample and the vacuum of the mass spectrometer. While polydimethylsilicone membranes have proven to be extremely suitable for real-time VOC analysis, other analytes and matrices pose technically challenging problems in the normal MIMS configuration. The proposed 3-year project will explore several areas to address these problems: improved membrane selectivity for sample introduction; the applicaiton of ion-molecule chemistry and advanced mass spectrometer operation to improve speciation of mixtures and complex aqueous samples; development of techniques for extraction of soil-bound contaminants; and the pursuit of derivatization methods to make MIMS amenable to heavy metal analysis. This science will lead to real-time mass spectroscopic methods that can be applied to a variety of problems in environmental characterization. We intend to collaborate with university researchers in this project, and plan to seek to establish formal collaborative relationships with industrial partners.

Membrane introduction mass spectrometry (MIMS) functions as a near real-time monitor: there is no sample preparation; sample analysis time is seconds to minutes; and the cost of an analysis would be perhaps 1/10 that of current methods. MIMS can be implemented as a flow injection technique; samples, standards, and method blanks can be sequentially analyzed in a continuous fashion. This provides a facile path to rigorous QA/QC documentation of method performance that is obtained nearly simultaneously with sample results. MIMS operates as a closed-loop system: the sample can be returned directly to the waste stream, thus mitigating the creation of further waste during the analysis. And because the mass spectrometer is never directly exposed to the sample - the membrane interface provides that barrier - the mass spectrometer is kept clean and if applied to the analysis of mixed waste, potentially free from radioactive contamination. These features provide enhanced personnel safety and risk reduction compared to analytical methods that require off-line sample handling. Our experience in MIMS as documented be refereed publications suggests that there is moderate technical risk and we will describe preliminary data to document the feasibility of MIMS for metal analysis.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-107	C-45	Long Term Treatment/Storage/Disposal Operations
§ RL-WM03	C-193	Solid Waste Storage and Disposal
§ RL-WM04	C-197	Solid Waste Treatment
§+ SR-SW02	C-285	Transuranic Waste Project
§+ SR-SW03	C-287	Mixed Low Level Waste Project
ID-HLW-101	C-29	High-Level Waste Pretreatment
NV214	C-53	Industrial Sites
+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
OR-43204	C-77	ORNL Bethel Valley Deactivation and Decommissioning
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
RF014	C-213	Industrial Zone Closure Project

Environmental Management Science Program Research in New Mexico

Los Alamos National Laboratory

59990-NM - Fundamental Chemistry, Characterization, and Separation of Technetium Complexes in Hanford Waste

Year of Award: 1997 **Amount of Award:** $730,000
Problem Area: High Level Waste
Science Category/SubCategory: Separations Chemistry / Technetium Chemistry and Separations
Principal Investigator: Dr. Norman C. Schroeder, 505-667-0967, nschroeder@lanl.gov
Major Collaborator(s): Dr. David L. Blanchard Jr. at Pacific Northwest National Laboratory
For More Information: http://www.doe.gov/em52/59990.html

Description Provided by Investigator:

Technetium, as TcO_4^-, is a mobile species in the environment. This characteristic, along with it long half-life, (^{99}Tc, $t\frac{1}{2} = 213,000$ a) makes techmetium a major contributor to the long-term hazard associated with low level waste (LLW) disposal. Thus, technetium partitioning from nuclear waste tanks at DOE sites (Hanford, etc.) may be required so that the LLW forms meet DOE performance assessment criteria. Technetium separations assume that technetium exists as TcO4 - in the tank waste. However, recent work with actual Hanford waste indicates that much of the technetium exists in a form other than TcO_4^- and that these unidentified technetium species are not readily converted to pertechnetate by oxidation.

Technetium was introduced into the tank wastes as pertechnetate anion. However, years of thermal and radiolytic digestion in the presence of organic material, including complexants such as EDTA, NTA, citrate, and oxalate, may have produced stable, reduced technetium chelate complexes. To successfully partition technetium from tank wastes, it will be necessary to either remove these species with a new process, or degrade them to TcO_4^- so that conventional pertechnetate separation schemes will be successful. The success of DOE's technetium management strategy lies in understanding the nature of its speciation in the tank wastes.

The research will develop the complexation chemistry of aqueous pertechnetate under reducing conditions. The four major goals of this research are to: (1) synthesize and characterize the major classes of technetium complexes formed under tank waste conditions, (2) study the ligand substitution and redox chemistry of these complexes, (3) use the complexes as standards for characterizing the non-pertechnetate species in actual waste using x-ray absorption spectroscopy (EXAFS and XANES) and for developing capillary electrophoresis mass spectrometry as a characterization technique, and (4) use the technetium complexes to develop efficient oxidation or separation methods for the non-pertechnetate species in actual wastes.

This information will enable the development of separation and/or feed adjustment chemistry that will efficiently remove technetium from the waste and enable DOE to fulfill its tank waste remediation mission.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§+ RL-TW04	C-169	Retrieval Project
§+ RL-TW05	C-173	Process Waste Support
§+ SR-HL01	C-249	H-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations

Environmental Management Science Program Research in New Mexico

Los Alamos National Laboratory

59993-NM - Dynamic Effects of Tank Waste Aging on Radionuclide-Complexant Interactions

Year of Award: 1997 **Amount of Award:** $540,000
Problem Area: High Level Waste
Science Category/SubCategory: Separations Chemistry / Catalyst Chemistry and Waste Treatment
Principal Investigator: Dr. Rebecca Chamberlin, 505-667-1841, rmchamberlin@lanl.gov
Major Collaborator(s): Dr. Jeffrey B. Arterburn at New Mexico State University
For More Information: http://www.doe.gov/em52/59993.html

Description Provided by Investigator:

The long-range objective of this project is to provide a scientific basis for safely processing high-level nuclear tank wastes for disposal. Our goals are to identify a means to prepare realistic simulant formulations for complexant-containing Hanford tank wastes, and then use those simulants to determine the relative importance of various organic complexants and their breakdown products on the partitioning of important radionuclides.

The harsh chemical and radiolytic environment in high-level waste tanks alters both the organic complexants and the metal species, producing radionuclide-chelator complexes that resist standard separation methods. A detailed understanding of the complexation reactions of the key radionuclides in tank wastes would allow for reliable, science-based solutions for high-level waste processing, but a key problem is that tank waste samples are exceedingly difficult to obtain, transport and handle in the laboratory. In contrast, freshly-prepared simulated wastes are safe and readily obtained, but they do not reproduce the partitioning behavior of actual tank waste samples.

For this project, we will first artificially age complexant-containing tank waste simulants using microwave, ultrasound, and photolysis techniques that can be applied in any standard laboratory. The aged samples will be compared to samples of actual Hanford tank wastes to determine the most realistic aging method, on the basis of the organic fragments present, and the oxidation states and partitioning behavior of important radionuclides such as ^{90}Sr, ^{99}Tc, and ^{239}Pu. Our successful completion of this goal will make it possible for scientists in academic and industrial laboratories to address tank waste remediation problems without the enormous costs and hazards associated with handling actual tank waste samples.

Later, we will use our simulant aging process to investigate the relative effects of chelator degradation products on the partitioning of important radionuclides from the waste. Using NMR-active labels in the chelators, we will use a combinatorial approach of generating multiple chelator fragments in a single experiment and then determining which, if any, of the fragments have a negative effect on the separations chemistry. Our successful completion of this goal will specifically identify the most problematic organic fragments in complexant-containing waste and provide the basis for developing successful treatment strategies for these wastes.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§+ RL-TW04	C-169	Retrieval Project
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations

Environmental Management Science Program Research in New Mexico

Los Alamos National Laboratory

59996-NM - Plutonium Speciation, Solubilization, and Migration in Soils

Year of Award: 1997 **Amount of Award:** $750,000
Problem Area: Remedial Action
Science Category/SubCategory: Actinide Chemistry / Actinide (Heavy Element) Chemistry
Principal Investigator: Dr. Mary Neu, 505-667-9313, mneu@lanl.gov
Major Collaborator(s): Dr. Richard G. Haire at Oak Ridge National Laboratory
For More Information: http://www.doe.gov/em52/59996.html

Description Provided by Investigator:

The DOE is currently conducting cleanup activities at its nuclear weapons development sites, many of which have accumulated plutonium (Pu) in soils for 50 years. There is scientific uncertainty about the levels of risk to human health posed by this accumulation and whether Pu is migrating from Federal reserves onto public lands. To properly control Pu migration in soils, better evaluate the public risk, and design effective remediation strategies, a fundamental understanding of Pu speciation, transport, and release mechanisms is critically needed. Key elements of this research are:

- Determination of Pu oxidation state(s) and speciation in pond sediments and select soil samples. It is widely believed that Pu in soils at Rocky Flats Environmental Technology Site (RFETS) is not mobile, yet detention ponds are needed to meet effluent water quality standards. The speciation of Pu in these soils will be valid for other sites and will increase our understanding of actinide environmental chemistry.

- The Pu concentrations in settling ponds show seasonal variation that correlate very well with Mn concentrations. Actual pond sediment samples collected on a seasonal basis will be used to evaluate the impact of mineral redox cycling on Pu solubility and mobility. Laboratory studies using synthetic Mn/Fe minerals and Pu species will be performed in parallel to determine the interaction mechanisms between Pu and these minerals and the potential change in Pu mobility due to redox cycling.

- Thermal Ionization Mass Spectrometry (TIMS) analysis to establish plutonium concentrations and distributions, and $^{240}Pu/^{239}Pu$ ratios in soils at RFETS, to better understand Pu pathways from contamination sources and to provide a critical basis to assess public risk from actinide migration. Concentrations and isotopic ratios of Pu in pond sediments as a function of depth will gauge changes in the Pu chemistry with time.

- Chemical systems important in Pu environmental behavior will be studied, providing critical thermodynamic data, as well as structural and chemical models for environmental samples. The Pu (III, IV, and V) species to be investigated will include: $Pu(CO_3)^+$, $Pu(OH)_x^{3-x}$, colloidal Pu(IV) hydroxide, $Pu(OH)_x(CO_3)_y^{4-x-2y}$, PuO_2^+ and $PuO_2CO_3^-$.

- Results of studies will provide data for control and prediction of Pu release, metal chemistry in groundwaters and soils, thermodynamic modeling, site decontamination, and risk assessment.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
+ RL-TW04	C-169	Retrieval Project
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
+ SR-HL02	C-253	F-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations

Environmental Management Science Program Research in New Mexico

Los Alamos National Laboratory

60015-NM - Long-term Risk from Actinides in the Environment: Modes of Mobility

Year of Award: 1997 **Amount of Award:** $900,020
Problem Area: Health / Ecology / Risk
Science Category/SubCategory: Biogeochemistry / Biogeochemistry
Principal Investigator: Dr. David D. Breshears, 505-665-2803, daveb@lanl.gov
Major Collaborator(s): Dr. Shawki Ibrahim at Colorado State University
Dr. Thomas Kirchner at New Mexico State University
For More Information: http://www.doe.gov/em52/60015.html

Description Provided by Investigator:

The mobility of actinides in surface soils is a key concern at several DOE facilities in arid and semiarid environments, including Rocky Flats, Hanford, Nevada Test Site, Idaho National Engineering and Environmental Laboratory, and Los Alamos National Laboratory and the Waste Isolation Pilot Plant (WIPP). Currently, Pu mobility is a high visibility issue at Rocky Flats and Hanford, with current litigation clean-up decisions pending on assessment of the risks resulting from the long-term mobility of Pu. Key sources of uncertainty in assessing Pu mobility are the magnitudes of mobility resulting from three modes of transport: (1) wind erosion, (2) water erosion, and (3) vertical migration. Each of these three processes depend on numerous environmental factors and they compete with one another, particularly for actinides in very shallow soils (~ 1 mm). The overall goal of the study is to quantify the mobility of soil actinides from all three modes. We propose to conduct a set of studies on four plots and obtain additional measurements at adjacent locations at each of three DOE facilities where actinide kinetics are of concern: Rocky Flats, Hanford, and WIPP. Tracers will be applied to plots and their redistribution will be measured over time. Wind erosion will be quantified using spatially-distributed aerosol measurements, including finely time-resolved measurements, and will be correlated with meteorological and ground cover conditions. Water erosion will be quantified using rainfall simulator experiments in the field to measure vertical and horizontal changes in the tracer distribution. Vertical migration will be studied using tracers on and off of the rainfall simulation plots and will be measure through time to quantify the effects of various biological and weathering processes. The results will be integrated using a modeling approach, building on existing code and modifying the predictions based on experimental results.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Health / Ecology / Risk problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Health / Ecology / Risk".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
ID-HLW-101	C-29	High-Level Waste Pretreatment
ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-TW05	C-173	Process Waste Support
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW08	C-185	Process Waste Privatization Infrastructure
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
+ SR-HL01	C-249	H-Tank Farm
SR-HL05	C-265	Vitrification
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in New Mexico

Los Alamos National Laboratory

60118-NM - Fundamental Thermodynamics of Actinide-Bearing Mineral Waste Forms

Year of Award: 1997 **Amount of Award:** $1,150,000
Problem Area: Nuclear Materials
Science Category/SubCategory: Materials Science / Chemical and Structural Properties Of Storage Materials
Principal Investigator: Dr. Mark A. Williamson, 505-667-4045, maw@lanl.gov
Major Collaborator(s): Dr. Bartley B. Ebbinghaus at Lawrence Livermore National Laboratory
Dr. Alexandria Navrotsky at the University of California at Davis
For More Information: http://www.doe.gov/em52/60118.html

Description Provided by Investigator:

The end of the Cold War raised the need for the technical community to be concerned with the disposition of excess nuclear weapon material. The plutonium will either be converted into mixed-oxide fuel for use in nuclear reactors or immobilized in glass or ceramic waste forms and placed in a repository. The stability and behavior of plutonium in the ceramic materials as well as the phase behavior and stability of the ceramic material in the environment is not well established. In order to provide technically sound solutions to these issues, thermodynamic data are essential in developing an understanding of the chemistry and phase equilibria of the actinide-bearing mineral waste form materials proposed as immobilization matrices. Mineral materials of interest include zircon, zirconolite, and pyrochlore. High temperature solution calorimetry is one of the most powerful techniques, sometimes the only technique, for providing the fundamental thermodynamic data needed to establish optimum material fabrication parameters, and more importantly understand and predict the behavior of the mineral materials in the environment. The purpose of this project is to experimentally determine the enthalpy of formation of actinide orthosilicates, the enthalpies of formation of actinide substituted zirconolite and pyrochlore, and develop an understanding of the bonding characteristics and stabilities of these materials.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Nuclear Materials problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Nuclear Materials".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ RL-TP07	C-161	Plutonium Finishing Plant (PFP) Vault Management
ID-HLW-101	C-29	High-Level Waste Pretreatment
ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
+ RL-TW05	C-173	Process Waste Support
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW08	C-185	Process Waste Privatization Infrastructure
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
+ SR-HL01	C-249	H-Tank Farm
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in New Mexico

Lovelace Biomedical & Environmental Research Institute

54940-NM - Improved Risk Estimates for Carbon Tetrachloride

Year of Award: 1996 **Amount of Award:** $1,000,000
Problem Area: Health / Ecology / Risk
Science Category/SubCategory: Health Science / Risk Assessment
Principal Investigator: Dr. Janet M. Benson, 505-845-1147, jbenson@lucy.tli.org
Major Collaborator(s): David L. Springer at Pacific Northwest National Laboratory
For More Information: http://www.doe.gov/em52/54940.html

Description Provided by Investigator:

Carbon tetrachloride (CCl_4) has been used extensively within the Department of Energy (DOE) nuclear weapons facilities. Costs associated with cleanup of CCl_4 at DOE facilities are driven by current cancer risk estimates which assume CCl_4 is a genotoxic carcinogen. However, a growing body of evidence suggests that CCl_4 is not genotoxic. In April 1996, the Environmental Protection Agency (EPA) published proposed new guidelines for cancer risk assessment. In the new guidelines, the agent's mode of action is considered, and conclusion of hazard may be made based on the route, duration, and magnitude of exposure. These proposed guidelines provide an opportunity to develop a broader, more scientifically based estimate of the human cancer risk associated with CCl_4 exposure. The overall purpose of these studies is to improve the scientific basis for assessing the cancer risk associated with human exposure to CCl_4. Specifically, we will determine the toxicokinetics of inhaled and ingested CCl_4 in F344/Crl rats, $B6C3F_1$ mice, and Syrian hamsters. We will also evaluate species differences in the *in vivo* metabolism of CCl_4 by rats, mice, and hamsters and the *in vitro* metabolism of CCl_4 by tissues and microsomes from these rodent species and man. Dose-response relationships will be evaluated in all these studies. This information will be used to improve the current physiologically based pharmacokinetic model for CCl_4. We will also determine whether $CC1_4$, like chloroform, is a hepatocarcinogen only when exposure results in cell damage, cell killing, and regenerative cell proliferation. In combination, the results of these studies will provide the types of information needed to enable a refined cancer risk estimate for $CC1_4$ under the EPA's proposed new guidelines for cancer risk assessment. Application of a revised cancer risk estimate for CCl_4 may result in less stringent levels for CCl_4 cleanup at DOE facilities, thereby significantly reducing associated costs to the DOE.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Health / Ecology / Risk problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Health / Ecology / Risk".

Environmental Management Science Program Research in New Mexico

Lovelace Biomedical & Environmental Research Institute

59918-NM - Improved Radiation Dosimetry/Risk Estimates to Facilitate Environmental Management of Plutonium Contaminated Sites

Year of Award: 1997 **Amount of Award:** $862,784
Problem Area: Health / Ecology / Risk
Science Category/SubCategory: Health Science / Biophysics/Dose
Principal Investigator: Dr. Bobby R. Scott, 505-845-1176, bscott@itri-1.lrri.org
For More Information: http://www.doe.gov/em52/59918.html

Description Provided by Investigator:

The Office of Environmental Management is the custodian of large quantities of toxic radioactive materials from manufacturing and processing facilities after the United States halted nuclear weapons production. Because these materials include high-specific activity (HSA) and low-specific activity (LSA) alpha-emitting (αE) isotopes of plutonium (Pu), DOE workers and the public can be at risk for inhaling airborne αE particles. Examples of HSA-αE particles are particles of $^{236}PuO_2$, $^{238}PuO_2$, and $^{240}PuO_2$. Examples of LSA-αE Pu particles are particles of $^{239}PuO_2$, $^{242}PuO_2$, and $^{244}PuO_2$. It is generally not recognized that airborne HSA-αE particles or mixtures of HSA-αE and LSA-αE particles present special problems for evaluating health-effects risks for workers involved in decontamination, decommissioning, and remediation. These problems arise because inadequate dosimetry models are used for characterizing the intake by inhalation of airborne HSA-αE particles and the associated local internal radiation doses. This inadequacy is especially unfortunate for those who may be at risk of inhaling HSA-αE particles when their airborne concentration is very low (much less than one particle per cubic meter of air). Such exposures are considered to be in the stochastic-exposure paradigm. For this paradigm, one cannot say whether anyone will inhale an HSA-αE particle. However, should an individual inhale even one HSA-αE particle, the radioactivity intake can exceed the annual limit for nuclear worker exposure (annual limit on intake). One HSA-αE particle could therefore represent a relatively large intake of radioactivity. Furthermore, HSA-αE particles are unstable due to the alpha-decay energy absorbed within the particle. If the particle is deposited in the respiratory tract, it can subsequently fragment into smaller particles leading to more surface area available for particle dissolution. Thus, radioactivity moves more rapidly from the respiratory tract to the liver and skeleton, via the blood, than occurs for LSA-αE particles. However, because no existing dosimetry model is adequate for evaluating possible radiation doses from inhalation of airborne αE particles for the stochastic-exposure paradigm, health risks from such exposures cannot be reliably evaluated. For these exposures to airborne αE particles and for the stochastic-exposure paradigm, it is preferable to evaluate the distribution of possible cancer risks rather than evaluating the risk associated with the expected intake of radioactivity because risk estimates based on expected intake can lead to wasting millions and possibly even more dollars on excessive cleanup of residual radioactivity. This project will apply fundamental knowledge of mechanisms of cancer induction, aerosol physics, and radiation dosimetry to: (1) evaluate αE particle inhalation/deposition probabilities for adult male and female workers and for different members of the public (children, teenagers, and adults of both sexes); (2) characterize HSA-αE particle breakup and its impact on translocation of radioactivity from the lung to the liver and skeleton; (3) evaluate deposition of α energy in biological tissues for stationary and moving αE particles; and (4) evaluate the distribution of possible doses to lung (local doses), bone (organ dose), and liver (organ dose) and associated cancer-risk distributions for specific αE particle exposure scenarios relevant to environmental management of sites contaminated with αE sources. The main product of this research will be a stochastic respiratory tract dosimetry/risk computer model for evaluating absorbed dose distributions and the associated health risks distributions. The research will contribute to building a stronger scientific basis for environmental management of Pu-contaminated sites and to substantially reducing cleanup costs for such sites by eliminating the need to evaluate health risks for the stochastic exposure paradigm based on the expected intake of radioactivity.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Health / Ecology / Risk problems, are listed in the <u>Index of High Cost Environmental Management Projects by Problem Area</u>, in the back of this appendix, under the heading "Health / Ecology / Risk".

Environmental Management Science Program Research in New Mexico

Sandia National Laboratories - Albuquerque

55332-NM - A Hybrid Hydrologic-Geophysical Inverse Technique for the Assessment and Monitoring of Leachates in the Vadose Zone

Year of Award: 1996 **Amount of Award:** $2,024,074
Problem Area: Remedial Action
Science Category/SubCategory: Geophysics / Subsurface Imaging
Principal Investigator: Dr. David L. Alumbaugh, 505-844-0555, dlalumb@sandia.gov
Major Collaborator(s): Jim Brainard at the University of Arizona
For More Information: http://www.doe.gov/em52/55332.html

Description Provided by Investigator:

It is the objective of this proposed study to develop and field test a new, integrated Hybrid Hydrologic-Geophysical Inverse Technique (HHGIT) for characterization of the vadose zone at contaminated sites. This fundamentally new approach to site characterization and monitoring will provide detailed knowledge about hydrological properties, geological heterogeneity and the extent and movement of contamination. HHGIT combines electrical resistivity tomography (ERT) to geophysically sense a 3D volume, statistical information about fabric of geological formations, and sparse data on moisture and contaminant distributions. Combining these three types of information into a single inversion process will provide much better estimates of spatially varied hydraulic properties and three-dimensional contaminant distributions than could be obtained from interpreting the data types individually. Furthermore, HHGIT will be a geostatistically based estimation technique; the estimates represent conditional mean hydraulic property fields and contaminant distributions. Thus, this method will also quantify the uncertainty of the estimates as well as the estimates themselves. The knowledge of this uncertainty is necessary to determine the likelihood of success of remediation efforts and the risk posed by hazardous materials. Controlled field experiments will be conducted to provide critical data sets for evaluation of these methodologies, for better understanding of mechanisms controlling contaminant movement in the vadose zone, and for evaluation of the HHGIT method as a long term monitoring strategy.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER02	C-129	200 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in New Mexico

Sandia National Laboratories - Albuquerque

55387-NM - Photooxidation of Organic Wastes Using Semiconductor Nanoclusters

Year of Award: 1996 **Amount of Award:** $1,251,000
Problem Area: Mixed Waste
Science Category/SubCategory: Materials Science / Surface Chemistry
Principal Investigator: Dr. J. P. Wilcoxon, 505-844-3939, jpwilco@sandia.gov
Major Collaborator(s): D. F. Kelley at Colorado State University
For More Information: http://www.doe.gov/em52/55387.html

Description Provided by Investigator:

Solar detoxification is a process wherein sunlight is captured by a semiconductor particle in suspension to create electrons and holes that then diffuse to the particulate surface to effect the oxidation and reduction of toxic pollutants. Using solar energy to oxidize organic chemicals to carbon dioxide and dilute mineral acids is very energy efficient compared to other methods such as incineration. Finding an efficient particulate has thus been a focus of research, which has had only limited success, the fundamental problem being that materials that efficiently absorb in the visible portion of the solar spectrum also photocorrode.

Past solar detoxification efforts have relied almost exclusively on titanium dioxide, and although it is photostable, it is a *white* material with a UV bandgap that absorbs less than 7% of the solar spectrum. It also suffers from electron-hole recombination in commercially available forms. Recent research has made possible the synthesis of photostable semiconductor nanoclusters with *visible* band gaps that can be tuned by adjusting the cluster size. Thus bulk materials with near IR absorbence edges can be made into visible band-edge materials with stronger redox potentials.

The rate of electron-hole recombination is small in nanoclusters, so they have the potential to act as highly efficient solar detoxification agents. In effect, they act more like molecular organic photoredox catalysts, but with significant advantages in chemical stability because they are inorganic. We propose to investigate the use of these materials in practical detoxification applications, using facilities already in place here at Sandia and at Colorado State University.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW03	C-287	Mixed Low Level Waste Project
AL024	C-3	Grand Junction Office (GJO) All Other Projects
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ OR-48101	C-99	Offsite Remedial Action
+ OR-45301	C-103	Paducah Remedial Action
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
RL-ER08	C-147	Groundwater Management
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in New Mexico

Sandia National Laboratories - Albuquerque

55395-NM - Physics of DNAPL Migration and Remediation in the Presence of Heterogeneities

Year of Award: 1996 **Amount of Award:** $1,245,000
Problem Area: Remedial Action
Science Category/SubCategory: Hydrogeology / Dense Non-Aqueous Phase Liquid (DNAPL) Dynamics
Principal Investigator: Dr. Stephen Conrad, 505-848-0759, shconra@nwer.sandia.gov
Major Collaborator(s): Robert Glass at Sandia National Laboratories - Albuquerque
For More Information: http://www.doe.gov/em52/55395.html

Description Provided by Investigator:

We will conduct well-controlled laboratory experiments to better understand the physics of DNAPL migration and remediation in the presence of heterogeneities. These experiments will be used to develop and test an upscaled percolation model, a new approach for modeling DNAPL migration. Finally, numerical simulators under current use in evaluating remediation techniques will be compared against our remediation experiments. We will make use of our unique experimental capabilities in the Subsurface Flow and Transport Processes Laboratory at Sandia to conduct controlled, systematic, repeatable experiments that first consider the physics of DNAPL migration in initially water saturated, heterogeneous porous media and then evaluate the efficacy of a suite of promising remediation techniques for remediating DNAPLs from heterogeneous aquifers. The results of the migration experiments will be used to test and continue development of new modeling approaches based on upscaled percolation theory developed by us and by collaborators. In addition, the results of the remediation experiments will be used to test, for the first time, within heterogeneous media the quantitative performance of remediation design codes (two-phase flow codes that incorporate compositional models).

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ OR-46301	C-107	Portsmouth Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in New Mexico

Sandia National Laboratories - Albuquerque

60363-NM - Optimization of Thermochemical, Kinetic, and Electrochemical Factors Governing Partitioning of Radionuclides during Melt Decontamination of Radioactively Contaminated Stainless Steel

Year of Award: 1997 **Amount of Award:** $1,200,000
Problem Area: Decontamination and Decommissioning
Science Category/SubCategory: Materials Science / Waste Materials
Principal Investigator: Dr. James A. Van den Avyle, 505-845-3105, JAVANDE@sandia.gov
For More Information: http://www.doe.gov/em52/60363.html

Description Provided by Investigator:

Melt Decontamination represents an effective scrap metal recycling route for the estimated 1,200,000 tons of contaminated stainless steel and nickel currently within the DOE complex. At present, this material must be considered a substantial disposal liability. However, with appropriate recycling, this material may be regarded as an asset worth an estimated $5 billion. The DOE anticipated buying 6.2 million tons of stainless steel for use as waste burial containers. The proposed outcome of this work would eliminate the need for many of those containers while providing the material for the remainder. The conversion of a disposal liability into a final product (which DOE already plans to purchase) reduces the volume of material necessary for burial and saves billions of dollars in material costs.

The goal of this project is to optimize a melt decontamination process through a basic understanding of the factors which govern the partitioning of various radionuclides between the metal, slag, and gas phases. Radionuclides which are captured by a slag phase may be stabilized by promoting the formation of synthetic minerals within a leach resistant matrix. This research describes an integrated program of simlulation and experimentation designed to investigate and optimize liquid metal techniques for the decontamination and recycling of radioactive scrap metal. This program will combine Sandia expertise and ongoing work in fundamental separation science and liquid metal processing technology via a focused effort aimed at understanding the thermodynamic, electrochemical, and kinetic reactions which occur within melt refining processes. The goal of this work is to apply a broad range of Sandia capabilities and experience towards the development of a viable method to decontaminate and recycle high value metals currently within the DOE complex, as well as stabilizing and significantly reducing the volume of radioactive contaminated waste in need of disposal. **While melt decontamination of radioactive contaminated metals has been previously studied, this work represents the first comprehensive effort to understand and optimize the driving forces which govern decontamination by means of radionuclide partitioning.**

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Decontamination and Decommissioning problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Decontamination and Decommissioning".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ OR-43204	C-77	ORNL Bethel Valley Deactivation and Decommissioning
§ OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
§+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
§+ RL-ER06	C-141	Decontamination and Decommissioning
§+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
§ RL-TP10	C-163	Accelerated Deactivation
+ OR-48101	C-99	Offsite Remedial Action
+ OR-45301	C-103	Paducah Remedial Action
RL-ER08	C-147	Groundwater Management
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
RF014	C-213	Industrial Zone Closure Project

Environmental Management Science Program Research in New Mexico

Sandia National Laboratories - Albuquerque

60403-NM - Phase Chemistry of Tank Sludge Residual Components

Year of Award: 1997 **Amount of Award:** $1,157,000
Problem Area: High Level Waste
Science Category/SubCategory: Geochemistry / Sorption/Desorption
Principal Investigator: Dr. James L. Krumhansl, 505-844-9093, jlkrumh@sandia.gov
Major Collaborator(s): Dr. Jun Liu at Pacific Northwest National Laboratory
Dr. Kathryn L. Nagy at the University of Colorado
For More Information: http://www.doe.gov/em52/60403.html

Description Provided by Investigator:

It will not be possible to recover all the contaminated sludge from the bottoms of decommissioned waste storage tanks. This research is directed at providing a credible model for the release of radionuclides from residual sludge. Sludge components that are the prime actors in retaining radionuclides will be identified and synthesized. Both sorption and desorption of the radionuclides will be addressed. AFM and STM studies will provide a firm atomistic explanation for the observed sludge-radionuclide-solution interactions. Finally, this understanding will be used to develop a quantitative radionuclide release source term for use in performance assessment calculations.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§ ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§+ RL-TW08	C-185	Process Waste Privatization Infrastructure
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§ SR-HL05	C-265	Vitrification
NV214	C-53	Industrial Sites
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in New Mexico

New Mexico Institute of Mining & Technology

54857-NM - Surface Nuclear Magnetic Resonance Imaging of Water Content Distribution in the Subsurface

Year of Award: 1996 **Amount of Award:** $637,740
Problem Area: Remedial Action
Science Category/SubCategory: Engineering Science / Diagnostics
Principal Investigator: Dr. Jan M.H. Hendrickx, 505-835-5892, hendrick@nmt.edu
Major Collaborator(s): Peter Joseph at the University of Pennsylvania
For More Information: http://www.doe.gov/em52/54857.html

Description Provided by Investigator:

The objective of this research is to advance the technology of nuclear magnetic resonance (NMR) for direct measurement of water content distributions in the subsurface. The proof-of-concept of this method has been demonstrated by Russian scientists at the Institute of Chemical Kinetics and Combustion at Novosibirsk, and more recently by the Israeli Institute of Petroleum Geology and Geophysics at Holon, Israel and at the company IRIS in France. We propose to make advances in three critical components of the technology: (1) Developing the 3-D inverse and forward models needed for processing and interpretation of field measurements; (2) Improvement of the design and prototype construction with commercially available electronic equipment; and (3) Testing of the computing algorithms and improved equipment at hydro geologically well characterized sites. Since the movement of many contaminants in the subsurface directly depends on the water content distribution, the proposed NMR research has the potential to greatly improve environmental risk assessments under a wide range of climatic conditions.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ AL007	C-7	Environmental Restoration
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV212	C-49	Underground Test Area (UGTA)
§ NV214	C-53	Industrial Sites
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER02	C-129	200 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in New Mexico

New Mexico Institute of Mining & Technology

55109-NM - New Permeameters for in situ Characterization of Unsaturated Heterogeneous Permeability

Year of Award: 1996 **Amount of Award:** $612,425
Problem Area: Remedial Action
Science Category/SubCategory: Hydrogeology / Instrumentation and Modelling
Principal Investigator: Dr. John L. Wilson, 505-835-5308, JWILSON@TAOS.NMT.EDU
Major Collaborator(s): Robert Glass at Sandia National Laboratories - Albuquerque
For More Information: http://www.doe.gov/em52/55109.html

Description Provided by Investigator:

Thick unsaturated zones underlie many DOE landfills, industrial areas, and waste storage sites in the western United States (U.S.) and are the primary pathway for contaminants to migrate into underlying aquifers. The spatial variability of unsaturated permeability in these heterogeneous geologic materials directly influences the movement of water and non-aqueous phase liquids (NAPL's), precluding meaningful modeling of contaminant transport for risk assessment or remediation design. In unsaturated materials, the influence of heterogeneity on flow and transport processes is amplified by capillary forces, because permeability is a function of both geologic heterogeneity and the fluid saturation. Poor characterization of heterogeneity may lead to ineffective remedial designs and increased risk, requiring subsequent additional remedial actions at increased cost and time. There are techniques that incorporate site-specific heterogeneity into a probabilistic risk framework for decision analysis, but they cannot be applied to the unsaturated zone with confidence. It is presently not possible to collect the large number of data they need to accurately define the spatial correlation structure of unsaturated permeability. Laboratory methods for estimating the unsaturated permeability are expensive, time-consuming, and may not yield results representative of heterogeneous field conditions. This project is aimed at the design, development and testing of new rapid, and cost effective field methods for estimating *in situ* unsaturated permeability.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ NV212	C-49	Underground Test Area (UGTA)
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in New Mexico

New Mexico Institute of Mining & Technology

60163-NM - Investigation of Techniques to Improve Continuous Air Monitors Under Conditions of High Dust Loading in Environmental Setting

Year of Award: 1997 **Amount of Award:** $309,650
Problem Area: Health / Ecology / Risk
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Sensors and Techniques
Principal Investigator: Dr. Stephen D. Schery, 505-835-5872, radon@jupiter.nmt.edu
For More Information: http://www.doe.gov/em52/60163.html

Description Provided by Investigator:

The investigation is an in-depth exploration of environmental influences that can cause degradation of the performance (sensitivity, alarm functionality, etc.) of Continuous Air Monitors (CAM's), such as the LANL/Canberra alpha-particle CAM, and a study of techniques to correct for this degradation. Such degradation is a subject of ongoing importance, especially since concerns about health effects associated with environmental radioactivity are leading to tighter and tighter controls on atmospheric releases of manmade radioactive substances. Degrading factors to be studied include ambient aerosol particulate deposits on CAM filters, and the interactions of radon progeny background, as well as plutonium or uranium, with such deposit structures. Making use of recently available time-lapse video microscopic technology, the formation of dendritic structures from aerosol loading will be studied on present LANL CAMs. In addition, New Mexico Tech has recently received from the University of Lund a research prototype pulsed ionization chamber with large surface area. The possibility of adapting such pulsed ionization chambers for innovative CAM use will be investigated. Their ability to monitor filters with areas five to ten times larger than in present CAMs might lead to a significant alleviation of the aerosol loading problem and improved sensitivity from increased air sampling flow rates. Findings from the project will be of significance for the design of CAM pre-separators, filter media and use, development of data analysis software, and other critical CAM design and operational issues. The outcome will be a more reliable, sensitive air monitoring instrument for environmental settings such as waste processing/disposal sites.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Health / Ecology / Risk problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Health / Ecology / Risk".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER06	C-141	Decontamination and Decommissioning
RL-TP10	C-163	Accelerated Deactivation
RF014	C-213	Industrial Zone Closure Project
+ SR-SW01	C-281	Consolidated Incinerator Facility

Environmental Management Science Program Research in New Mexico

New Mexico State University

54639-NM - Development of an In-Situ Microsensor for the Measurements of Chromium and Uranium in Groundwater at DOE Sites

Year of Award: 1996 **Amount of Award:** $690,000
Problem Area: Remedial Action
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Sensors and Techniques
Principal Investigator: Dr. Joseph Wang, 505-646-2140, joewang@nmsu.edu
Major Collaborator(s): Khris B Olsen at Pacific Northwest National Laboratory
For More Information: http://www.doe.gov/em52/54639.html

Description Provided by Investigator:

The goal of this program is to develop, optimize and deploy a silicon-based micromachined stripping analyzer for field monitoring trace levels of chromium and uranium. Such system will integrate the sample-handling steps and necessary chemical reactions (using a flow-injection operation) with the already proven adsorptive-stripping voltammetric operation on a small planar chip. Besides the drastic reduction in the size of the analytical system, such miniaturization should lead to increased speed, minimal reagent consumption and disposal, higher sensitivity and improved precision, and would thus revolutionize the way by which toxic metals are being monitored.

In order to fully exploit this opportunity, it will be necessary first to develop a fundamental understanding of the behavior of such scaled-down flow-injection stripping system. Considerations of proportionalities and similarity will thus be used for deriving theoretical expressions for the dependence of the response upon variables to be miniaturized. The new knowledge will serve as a useful guideline for the rational design of the system manifold, and through the optimization, characterization and field deployment of the micromachined analyzer. Overall, this research will create powerful and economical microsystems for in-situ monitoring of metal contaminants in DOE sites, and will shed useful insights into the micromachining and behavior of miniaturized flow analyzers, in general.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ AL007	C-7	Environmental Restoration
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV212	C-49	Underground Test Area (UGTA)
§ NV214	C-53	Industrial Sites
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER02	C-129	200 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ RF014	C-213	Industrial Zone Closure Project
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW05	C-173	Process Waste Support
+ RL-TW07	C-181	Process Waste Privatization Phase II
+ SR-HL01	C-249	H-Tank Farm
+ SR-HL02	C-253	F-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
SR-HL05	C-265	Vitrification
+ SR-SW01	C-281	Consolidated Incinerator Facility

Environmental Management Science Program Research in New Mexico

New Mexico State University

54823-NM - Modeling of Cation Binding in Hydrated 2:1 Clay Minerals

Year of Award: 1996 **Amount of Award:** $359,422
Problem Area: Remedial Action
Science Category/SubCategory: Geochemistry / Sorption/Desorption
Principal Investigator: Dr. David E. Smith, 505-646-5210, davsmith@nmsu.edu
For More Information: http://www.doe.gov/em52/54823.html

Description Provided by Investigator:

Hydrated 2:1 clay minerals are high-surface area, layered silicates that play a unique role in determining the fate of ionic pollutants in the environment. These minerals, including smectites and vermiculites, make up a major component of many soils. Ionic pollutants, including radioactive metal ions, may displace interlayer cations from the clay and bind, sometimes irreversibly, to the fixed-charge sites on the clay layer sheets. This binding in turn has a significant impact on pollutant transport through soils and clay-based containment materials, and on groundwater and soil remediation strategies. The molecular mechanisms whereby cations bind to 2:1 clay minerals are, unfortunately, not fully understood. The compositional variability of clays, particularly the magnitude and location of isomorphic substitution sites, has a significant impact on their binding properties. In addition, the complicated balance between hydration forces and ion-clay interactions is often difficult to quantify. The general goal of our research is to develop molecular models for cation binding to clays through the use of computer simulations. These models will build our intuition into cation-clay binding phenomena while explicitly identifying the key elements in the interactions that account for observed binding behavior. This in turn will assist in predicting and understanding the distribution coefficients that are used to model pollutant transport through natural soils or containment materials. In addition, strategies for soil remediation will benefit from an improved fundamental understanding of the nature of the binding interactions.

The production of nuclear weapons during the cold-war era led to the creation of enormous amounts of radioactive waste materials. Many of these wastes were stored improperly, leading to seepage or massive discharges into the soil and groundwater. At other times, waste was intentionally discharged directly into the environment. Many questions now exist regarding the fate of radioactive waste products that are present in the soil and groundwater. How fast and by what mechanisms do these wastes move? How and when might they be transported into the biosphere? How can contaminated soil best be isolated or remediated?

The transport of radioactive ions through subsurface environments is a complicated process that depends on a variety of compositional and chemical variables. It is clear, however, that transport often depends explicitly on cation binding affinities to clays. For example, cesium ions have a higher binding affinity for some 2:1 clay minerals than do strontium ions. As a result, strontium moves more quickly through soils than does cesium. The binding of cesium is non-linear with cesium concentration, indicating the presence of a few very-strong binding sites. It has been speculated that these binding sites are ditrigonal cavities, yet this has not been demonstrated directly. The specific role of layered silicates in binding divalent cations such as strontium is also the subject of some debate. The studies we propose here should help to elucidate the molecular mechanisms of cation binding.

Issues involving the proper storage and isolation of spent fuel, high-level waste, and transuranic waste are also subjects of intense current research and development. Radioactive wastes are unique among pollutants in that they cannot be destroyed in the traditional sense --radioactive nuclei remain radioactive until they spontaneously decay (or are forced to decay in nuclearreactors). Many radioactive isotopes have half-lives of thousands or millions of years. As a result, long-term storage and isolation technologies must be developed before waste can be removed from temporary storage facilities now in operation. Current strategies for long-term storage of nuclear waste involve geological repositories such as the Waste Isolation Pilot Plant in New Mexico and the proposed Yucca Mountain site in Nevada. One key feature of geological repositories is the use of containment and backfill materials that can provide a sealing and sorbing buffer to radionuclide transport. Hydrated 2:1 clays, particularly smectites, are characterized by their tendency to swell when exposed to water. This leads to a 'self-sealing' behavior and slow transport of water and pollutants through compacted clays. The combination of swelling and adsorption properties makes smectites primary candidates for containment and backfill materials. Further studies of radionuclide transport through compacted clays is required, however, to validate the long-term effectiveness of these materials. Building a molecular understanding of cation binding and diffusion in these materials will assist in this process.

We propose specifically to investigate the molecular origin of cation binding and mobility in hydrated clay minerals using simulation techniques. Computer simulations assist directly in building molecular intuition into chemical systems and provide a bridge between experiment and theory. Simulation models have been developed recently for investigations of clay hydration structures and basal spacings. To date, however, no calculations of cation binding thermodynamics have been reported.

Our simulations will be used to build a molecular-level understanding of cation binding, and to analyze theories for cation exchange in clays. Specific focus will be given to cesium (Cs^+), strontium (Sr^{2+}), and uranium(VI) ($UO_2{}^{2+}$ and hydrolysis products) cations, in that order, and to smectite and vermiculite clays of varying composition. The ions are chosen because they are important ionic components of high-level waste (Cs^+ and Sr^{2+}) and spent fuel ($UO_2{}^+$). Each of the ions are common radioactive contaminants present in groundwater and soils (uranium being the most common). Accurate simulation models for aqueous cesium and strontium solutions have been developed recently by us. A first-generation model for simulations of aqueous $UO_2{}^{2+}$ solutions has also been developed recently, although accurate modeling of uranyl hydration and binding will require development of more sophisticated models that account for uranyl speciation as a function of pH. Variations in clay composition are a crucial feature of the research because the magnitude and location (tetrahedral -vs- octahedral layer) of the fixed-charge sites have a dramatic impact on cation binding to clays. One major goal of this research is the prediction of adsorption properties for individual clays directly from their molecular structure. This would directly impact radionuclide transport modeling in which binding constants serve as input parameters.

Existing theories to explain cation binding thermodynamics have been reviewed recently. Some theories are based upon an electrostatic description of ion hydration and binding, while others extend to include polarization effects in the context of hard and soft acid and base theory. Our simulations will provide a specific test of these theories by correlating exchange free energies with interlayer ion and water structures, degrees of hydration, clay basal spacing, and the nature of the clay-ion-water interactions.

Finally, our simulations will be used to investigate radionuclide transport through compacted clay materials, as might be found in nuclear waste repositories. The low permeability of compactedclays makes diffusion the principle mechanism for radionuclide transport. Simulation results will be compared with recent experimental measurements, some of which have raised questions regarding the specific mechanism of cation diffusion.

Much of the research herein stretches the boundaries of existing computer modeling capabilities. The currently available clay-ion-water models have provided successful descriptions of ion hydration and swelling behavior in a variety of alkali-metal substituted clays. In contrast, little modeling work has been done on multivalent cation-clay systems. A proposal to validate our methods and models for calculations of monovalent cation exchange has been funded by the ACS Petroleum Research Fund. It involves the calculation of exchange free energies for the alkali-metal ion series in a clay designed to mimic Llano vermiculite (VTx-1). This particular clay system is well-characterized experimentally in terms of both exchange thermodynamics and hydrated structure. The experimental data on this system will provide a necessary validation of the methods and interaction models used in the simulations, laying an important foundation for the investigations here.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

Environmental Management Science Program Research in New Mexico

University of New Mexico

54595-NM - f-Element Ion Chelation in Highly Basic Media

Year of Award: 1996 **Amount of Award:** $499,998
Problem Area: High Level Waste
Science Category/SubCategory: Actinide Chemistry / Actinide (Heavy Element) Chemistry
Principal Investigator: Dr. Robert T. Paine, 505-277-1661, rtpaine@unm.edu
For More Information: http://www.doe.gov/em52/54595.html

Description Provided by Investigator:

Technical Background

The U.S. Department of Energy (DOE) is faced with the formidable task of developing techniques for the safe and cost effective remediation of ~ $1.5 \times 10^7 ft^3$ of high level waste (HLW) stored in the DOE complex. Only a small fraction of the waste contains radioactive elements, but these species are responsible for most of the problems inherent in the handling and long term storage of the waste. The dominant emitters are cesium-137 and strontium-90; however, technetium and actinide species (Np, Pu, Am, Cm) are also significant contributors. Most of the waste containing these elements was originally handled in concentrated nitric acid media during reprocessing efforts. However, in order to reduce corrosion during temporary storage in large metal tanks, the solutions were made strongly alkaline. In addition, the reprocessing efforts introduced a number of complex inorganic (e.g., CO_3^{2-}) and organic (e.g., BPh_4^-) ions, chelating agents (e.g., EDTA), and solvents. As a result, the radioactive elements in many storage tanks (e.g., at the Hanford facility) exist in complex and variable solid and liquid matrices.

It has been proposed that the permanent disposal of the waste will require partitioning of the low and high activity components while minimizing their volumes, particularly for the HLW fraction. The initial treatment will likely involve physical separation of the solid and liquid fractions, and there may be some washing of the solid fraction. It is anticipated that the liquid fractions will contain small concentrations of individual radioactive elements with totally unknown speciation. The majority of the radioactive elements in the HLW will appear in the solids fraction, again with unknown speciation. It may prove possible to directly handle the solid fraction with existing or planned solid waste immobilization concepts; however, the liquid waste will likely require further chemical processing and separations.

General Technical Needs

It appears that existing liquid phase separation techniques, derived primarily for actinide (An) ions in acidic media, will not provide for satisfactory partitioning of radioactive elements from the alkaline HLW matrix. Vastly improved methods and approaches suitable for basic media will be required. Unfortunately, there does not exist a well-developed molecular chemistry knowledge base to support the derivation of new separations. As pointed out in the program announcement, one of the most vexing problems in designing advanced separations schemes for these alkaline matrix wastes is the general lack of information on fission product and An element chemical speciation in strongly basic media. Some detailed information is available for carbonate-rich media; however, much less is known about hydroxide-rich systems. Based upon what is known about the alkaline solution chemistry for these elements and several related stable transition metals (e.g., Fe), it can be assumed that a variety of complex, polynuclear oxide-hydroxide species will be present. Some of these species may be soluble in basic media, and the solubility may be enhanced by the presence of complexants (e.g., EDTA, carboxylates, polyphosphates).

It is clear that more information will be required in order to develop the necessary chemical separations. In particular, needs exist for detailed speciation studies of An elements in basic tank waste simulant media. We will *not* study this topic directly, since it will be addressed by research groups at the national laboratories who are equipped to handle radioactive elements. We will, however, study the speciation of several fission product elements that are present in the waste and also are adequate chemical models for the radioactive An elements. Additionally, it will be necessary to gather data on the interactions of various ligands with the metal species present in the soluble fraction, sol fraction and insoluble fraction of the waste system. Finally, there is need for developing new ligand systems that may serve to selectively bind and separate individual ions from the various alkaline waste fractions. As will be described below, our program will address these fundamental scientific needs. The information gained will contribute to the future development of improved extractants and solid waste washing agents. These advances will, in turn, be integral to the development of required, improved waste handling protocols.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§+ RL-TW04	C-169	Retrieval Project
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
§ SR-HL05	C-265	Vitrification
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
RF014	C-213	Industrial Zone Closure Project

Environmental Management Science Program Research in New York

Mechanical Technology, Incorporated

60040-NY - Development of Monitoring and Diagnostic Methods for Robots Used in Remediation of Waste Sites

Year of Award: 1997 **Amount of Award:** $402,782
Problem Area: Decontamination and Decommissioning
Science Category/SubCategory: Engineering Science / Robotics
Principal Investigator: Mr. Joseph Tecza, 518-785-2355, jtecza@mechtech.com
Major Collaborator(s): I. D. Walker at Rice University
For More Information: http://www.doe.gov/em52/60040.html

Description Provided by Investigator:

In the Environmental Restoration and Waste Management Program of the Department of Energy (DOE), extensive use of robots is planned for safe and efficient clean up of hazardous and radioactive waste sites. Robots operating at these waste sites will be exposed to a variety of life-limiting environmental and operational conditions. Undetected faults in these robots can have serious consequences including damage to the waste containment facilities by the faulty robot, complete or partial failure of the robots which could result in delays in the clean up activities, or in extreme cases could result in loss of the robot.

In this research proposal, to avoid the dangers associated with in-operation failure of robots, Mechanical Technology Inc. (MTI) and Rice University (RU) propose to develop Monitoring and Diagnostic (M&D) methods which would provide for early stage detection, isolation, and tracking of developing faults before they result in serious failure. Efficient M&D methods developed in this research would help the DOE personnel in reducing the risk of catastrophic in-site robot failures and thereby decrease the risk of damaging the containment facilities, loss of robot, and mission failures. By avoiding the additional time and cost required for post-robot-failure clean up, the M&D methods will help in providing for faster, safer, and less expensive clean up.

To perform M&D of robots, presently there are several applicable methods available in the literature which have been proven to provide early detection of incipient faults. However, all of these methods are limited in application to electrically driven robots. The utility and effectiveness of these methods in application to remediation robots, which are typically hydraulic in nature, have never been proven. The research in this program will be a pioneering effort for developing efficient M&D methods for hydraulic robots, with applications to a wide variety of robots including remediation robots, multi-arm manipulators, and industrial robots.

The work in this program is based on the extensive study undertaken in a different DOE program to analyze the M&D needs of remediation robots. In this study, the Rosie Mobile Worksystem, developed by RedZone Robotics and Carnegie Mellon University for operation in nuclear environments was selected as a reference. A failure modes and effects analysis was performed to identify various failure modes due to environmental and operational conditions, their cause and effect on the overall system performance, and the criticality, speed, and probability of failures. This analysis indicated that faults in the Hydraulic Power Supply Subsystem (HPSS) and the Tether Drive Subsystem of Rosie were the most critical for which M&D methods are needed. In the research, these M&D methods will be developed by assembling a test rig at MTI test laboratories for performing seeded-fault experiments. This test rig will be composed of a HPSS and an Actuator Subsystem which is representative of most of the typical actuators in Rose. A variety of faults originating due to radiation, corrosion, dust, fluid contamination, etc. will be installed in the test rig, and signals from nine different sensors will be used to provide early detection of faults.

To develop efficient M&D methods for remediation robots, the research will address two main challenges: (1) effective differentiation of changes in sensor signals due to faults from those due to robot dynamics in presence of noise and fault signature variability, and (2) quantification of the complex interactions between various components for fault isolation. The dynamic operation of the robot changes the sensor signals making it difficult to distinguish these changes from those caused by a fault. The task is further complicated by external noise in the sensor signal and fault signature variability due to the complex interactions between the robot and its environment. The research will investigate various dynamic model-based methods, fuzzy and dynamic thresholding methods, and pattern classification methods that can provide clear and early indication of faults in the robot by coping with robot dynamics, sensor noise, and fault signature variability. The second challenge the research will address relates to the complex interactions between various components in the robot and its environment that causes problems in differentiating the faulty components from their secondary effects. In the research, various expert system approaches based on fault trees and fuzzy knowledge representation will be investigated to identify the most effective means of identifying faults in remediation robots.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Decontamination and Decommissioning problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Decontamination and Decommissioning".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
§+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
§+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
+ RL-TP07	C-161	Plutonium Finishing Plant (PFP) Vault Management

Environmental Management Science Program Research in New York

Brookhaven National Laboratory

59982-NY - Reactivity of Peroxynitrite: Implications for Hanford Waste Management and Remediation

Year of Award: 1997 **Amount of Award:** $700,000
Problem Area: High Level Waste
Science Category/SubCategory: Separations Chemistry / Catalyst Chemistry and Waste Treatment
Principal Investigator: Dr. Sergei Lymar, 516-344-4333, lymar@bnl.gov
For More Information: http://www.doe.gov/em52/59982.html

Description Provided by Investigator:

Favorable conditions exist in Hanford solid and liquid waste for radiation-induced generation of peroxynitrite, a very powerful oxidizing and nitrating agent. A comprehensive series of fundamental studies is designed to provide mechanistic and quantitative appreciation of the contribution of peroxynitrite in the waste chemistry, which is presently not understood. These studies will include:

1. Determination of the radiochemical yields of peroxynnitrite generated in chemical mixtures simulating the various phases (salt cake, slurry, supernatant) of radioactive waste;

2. Through mechanistic studies of metal- and CO_2-catalyzed oxidations by peroxynitrite, estimation of the extent of peroxynitrite-mediated oxidative degradation of waste organic components;

3. Exploration of the feasibility of using controlled catalytic oxidation by peroxynitrite in remediation to destroy waste organic components, and to remove chromium from the waste sludges which would greatly increase waste compatibility with vitrification-based disposal technologies.

The results of these studies will contribute to better understanding of the radioactive waste chemistry and thereby to more informed decisions concerning disposals options and technologies.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§+ RL-TW04	C-169	Retrieval Project
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations

Environmental Management Science Program Research in New York

Columbia University

55100-NY - Human Genetic Marker for Resistance to Radiations and Chemicals

Year of Award: 1996 **Amount of Award:** $751,020
Problem Area: Health / Ecology / Risk
Science Category/SubCategory: Health Science / Molecular, Structural and Genomic Science
Principal Investigator: Dr. Howard B. Lieberman, 212-305-9241, lieberman@cuccfa.ccc.columbia.edu
For More Information: http://www.doe.gov/em52/55100.html

Description Provided by Investigator:

The overall objective of this research is to characterize the human RAD9 gene at molecular and cellular levels, and use the information and materials gained to develop a predictive assay for assessing risks posed to individuals involved in toxic waste clean-up.

Fission yeast Schizosaccharomyces pombe rad9 plays a key role in promoting radioresistance and chemoresistance since cells containing a mutation in this gene are highly sensitive to physical and chemical agents that damage DNA. Furthermore, rad9 mutant cells cannot delay cycling in early S phase or in G2 after incurring a block in DNA replication or DNA damage, respectively (i.e., they lack the early S phase and G2/M checkpoint controls). The inability to delay cycling appropriately is thought to be at least partially responsible for mutant sensitivity to DNA damaging agents, as the lack of checkpoints results in attempts to enter and complete mitosis in the presence of damaged DNA. The rad9 gene also regulates the activity of at least one DNA repair enzyme, SPDE, which is involved in repair of DNA damaged by UV light. Thus, rad9 mediates resistance to DNA damaging agents via cell cycle dependent, i.e., checkpoint control, and independent mechanisms.

In this proposal, we focus on the analysis of a recently isolated human structural homologue of S. pombe rad9, capable of partially rescuing the hyrdoxyurea sensitivity, radiosensitivity and related checkpoint control defects of rad9 null yeast. The following specific aims are designed to address the structure, function and regulation of this human RAD9, as well as to establish RAD9 as a tool to assess predisposition towards the development of deleterious health effects associated with exposure to radiations and chemicals. Given the significant role that fission yeast rad9 plays in radioresistance and chemoresistance, it is highly likely that RAD9 also has an important role in humans.

The following are the specific aims of the project, which focus on human RAD9:

1. Molecular characterization of human RAD9

    a. Isolation and structure of the genomic version of human RAD9
    b. In vitro mutagenesis to assess structure/function relationships
    c. Expression in cells and tissues to assess regulation

2. Determining the role of human RAD9 in radio/chemoresponsiveness and cancer

    a. Creation and characterization of human RAD9 mutant cells
    b. The status of RAD9 in cervical cancer cells and other types of cancers and genetic disorders

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Health / Ecology / Risk problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Health / Ecology / Risk".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
OR-43204	C-77	ORNL Bethel Valley Deactivation and Decommissioning
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation

Environmental Management Science Program Research in New York

Cornell University

54793-NY - Establishing a Quantitative Functional Relationship Between Capillary Pressure Saturation and Interfacial Area

Year of Award: 1996 **Amount of Award:** $961,753
Problem Area: Remedial Action
Science Category/SubCategory: Hydrogeology / Instrumentation and Modelling
Principal Investigator: Dr. Carlo D. Montemagno, 607-255-2280, cdm11@cornell.edu
Major Collaborator(s): Michael Celia at Princeton University
William Gray at the University of Notre Dame
For More Information: http://www.doe.gov/em52/54793.html

Description Provided by Investigator:

Through an integrated and focused research program that is comprised of theoretical, computational and experimental efforts this research effort is directed at: (1) improving on newly developed laboratory techniques to quantify and directly measure the functional relationship between phase interfacial area (a), saturation (S) and capillary pressure (P_c); (2) developing new computational algorithms in conjunction with laboratory measurements to predict P_c, S, and a; (3) testing exciting theory and developing new theory to describe the relationship between Pc, S and a at the large scale; and (4) synthesizing the results of the experimental, computational and theoretical investigative efforts to develop a genetic model based upon an intrinsic soil metric to describe the functional dependence of P_c, S, and a. The results of this research could be used to generate a site specific soil moisture characteristic surface. Ultimately the results of this research could served as the foundation upon which the true health and safety risk of site could be evaluated, the applicability of various remediation technologies examined, and the performance of implemented treatment strategies controlled.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ NV212	C-49	Underground Test Area (UGTA)
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
SR-HL03	C-257	Waste Removal Operations and Tank Closure

Environmental Management Science Program Research in New York

New York University School of Medicine

59882-NY - Measurements of Radon, Thoron, Isotopic Uranium and Thorium to Determine Occupational & Environmental Exposure & Risk at Fernald Feed Materials Production Center

Year of Award: 1997 **Amount of Award:** $630,000
Problem Area: Health / Ecology / Risk
Science Category/SubCategory: Health Science / Biophysics/Dose
Principal Investigator: Dr. Naomi H. Harley, 212-263-5287, harlen01@MCRCR6.MED.NYU.ED
For More Information: http://www.doe.gov/em52/59882.html

Description Provided by Investigator:

The research at the Fernald Environmental Restoration Management Corporation (FERMCO) site will provide radionuclide data, and realistic risk evaluation for isotopic radon, thorium, uranium and lead exposure.

We have developed and tested a passive radon monitor with proven accuracy and precision that can be miniaturized to provide accurate personal exposure during remediation. These monitors will be used in areas and personal exposure assessment.

We have a novel aerosol particle sampler that can provide measurements of the particle size distribution over long time periods (days to weeks). This will be the first remediation to provide personal and area particle size distribution measurements. The aerosol particle size is the major determinant in lung dose variability.

There was historic occupational and environmental exposure to ^{222}Rn. There will be exposure to ^{228,226}Ra, ^{220,222}Rn,^{228,230,232}Th, and ^{210}Pb during remediation. There are 2 silos containing 4000 Ci of ^{226}Ra which will undergo some form of vitrification. There are 8 waste pits containing radium, thorium and lead in particulate form with concentrations to 4000 pCi/g. These particulates will be airborne as material is resuspended during the excavation procedures. Our study will provide accurate personal exposure assessment for all of the hazardous procedures with data available throughout each process so that rapid decisions concerning risk can be made. On site and remote soil, water and air samples will provide a full delineation of the environmental radionuclide contamination. A realistic carcinogenic risk assessment, based on these extensive environmental and occupational measurements, will be available throughout the restoration.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Health / Ecology / Risk problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Health / Ecology / Risk".

Environmental Management Science Program Research in New York

Syracuse University

55179-NY - Acoustic Probe for Solid-Gas-Liquid Suspensions

Year of Award: 1996 **Amount of Award:** $750,841
Problem Area: High Level Waste
Science Category/SubCategory: Engineering Science / Diagnostics
Principal Investigator: Dr. Lawrence L. Tavlarides, 315-443-1883, dsbrown@summon.syr.edu
Major Collaborator(s): Margaret Greenwood at Pacific Northwest National Laboratory
For More Information: http://www.doe.gov/em52/55179.html

Description Provided by Investigator:

Treatment of the radioactive waste stored in tanks across the DOE complex will require real-time characterization and monitoring of the size and volume fraction of solids in slurries during retrieval, immobilization, and closure stages of waste processing. Acoustic probes have been shown to be quite effective in determining the solid content in solid-liquid suspensions. However, the presence of small amounts of gas present in the waste slurries formed, for example, by radiolytic degradation processes prevent the straightforward application of these probes to the waste slurries. The research will develop an acoustic probe for monitoring particle size and volume fraction in slurries both in the absence and the presence of gas bubbles. This will be accomplished by selecting the range of frequencies of acoustic waves for which the interference caused by the bubbles is minimal and by developing a theory for the acoustic wave propagation in solid-gas-liquid systems. The initial theoretical and experimental studies will be devoted to relatively well characterized three-phase systems to establish firmly the theory and the development of the probe. The latter studies will be devoted to more complex suspensions whose properties are similar to those encountered in various waste processes at the Hanford Site.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

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Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§+ RL-TW04	C-169	Retrieval Project
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
§ SR-HL05	C-265	Vitrification
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
RF014	C-213	Industrial Zone Closure Project
+ SR-SW01	C-281	Consolidated Incinerator Facility

Environmental Management Science Program Research in Ohio

Ohio State University

54585-OH - Permanganate Treatment of DNAPLs in Reactive Barriers and Source Zone Flooding Schemes

Year of Award: 1996 **Amount of Award:** $351,231
Problem Area: Remedial Action
Science Category/SubCategory: Geochemistry / Sorption/Desorption
Principal Investigator: Dr. Frank W. Schwartz, 614-292-6196, frank@geology.ohio-state.edu
Major Collaborator(s): Hubao Zhang at Intera, Incorporated
For More Information: http://www.doe.gov/em52/54585.html

Description Provided by Investigator:

RESEARCH OBJECTIVES

The goals of this study are (1) to elucidate the basic mechanisms by which potassium permanganate oxidizes common chlorinated solvents, various constituents in aqueous solution, and porous-medium solids, and (2) to assess the potential for chemical oxidation by potassium permanganate to serve as a remedial scheme involving either source zone flooding or reactive barriers. The research is a combined experimental/modeling study that builds on our extensive previous work in the area of reactive barrier systems, and modeling of reactive contaminant transport. The specific objectives of this study are (1) to describe through batch experiments the kinetics and mechanisms by which potassium permanganate oxidizes dissolved tetrachloroethene (PCE), trichloroethene (TCE), and dichloroethene (DCE), (2) to examine using column studies the nature and kinetics of reactions between potassium permanganate, residual DNAPLs (PCE, TCE, and DCE) and porous medium solids, (3) to represent the process understanding in flow and transport models that demonstrate the potential applicability of the approach, and (4) to apply the resulting computer code in the development of appropriate field tests for assessing the approach.

BACKGROUND AND SIGNIFICANCE

The contamination problems posed by chlorinated solvents are well known. When dissolved in contaminant plumes, solvent concentrations, chlorinated solvents pose an extremely difficult challenge for hydrogeologists attempting to remove them from the subsurface. First, even low aqueous concentrations could be greatly in excess of the public drinking-water standards, although many chlorinated solvents are sparingly soluble in water. Thus, a large volume of groundwater can be contaminated by a small volume of spilled solvent. Secondly, due to their stability and persistence in the subsurface, pools and residual solvents can remain over many decades, or even centuries and serve as a long-term source of continued groundwater contamination. Finally, chlorinated solvents typically do not move along the flow gradient in aquifers because they are denser than water and tend to move downward under a separate hydraulic head.

The Department of Energy has an important stake in research related to the clean up of chlorinated solvents at its many contaminated sites. The main motivation for research is that some conventional schemes (like pump-and-treat or in situ bioremediation) have limitations in dealing with solvent contamination. For example, the undetected presence of DNAPL at a site generally relegates pump-and-treat schemes to an effort in hydraulic plume control rather than mass recovery. Bioremediation schemes suffer because aerobic bacteria cannot use chlorinated aliphatic compounds as a primary substrate. Research (e.g., Savannah River Integrated Demonstration) is now focusing on schemes involving the cometabolism of compounds by stimulating the growth of methanogens. Chlorinated solvents such as TCE dissolved in contaminant plumes be transformed by organisms that use a primary substrate, such is methane, for metabolism. To date, formidable challenges remain in developing this approach for practical use. Other conventional approaches like soil vapor extraction and gas sparging work well when site conditions are appropriate. In summary, there remains a need for research to develop approaches to treat contamination due to both free phase and dissolved solvents.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

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Project ID	Page #	Project Title
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ OR-46301	C-107	Portsmouth Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Ohio

University of Cincinnati

54674-OH - Design and Development of a New Hybrid Spectroelectrochemical Sensor

Year of Award: 1996 **Amount of Award:** $850,000
Problem Area: High Level Waste
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Sensors and Techniques
Principal Investigator: Dr. William R. Heineman, 513-556-9210, William.Heineman@UC.Edu
Major Collaborator(s): Samuel A Bryan at Pacific Northwest National Laboratory
For More Information: http://www.doe.gov/em52/54674.html

Description Provided by Investigator:

The required remediation of over 300 underground nuclear waste storage tanks at USDOE sites together with the associated needs to characterize and monitor the chemical compositions of the tanks themselves presents a major scientific challenge. In addition to the previously identified chemical complexity of such storage materials, the added dimensions of limited tank access and harsh chemical and radiological environment preclude the straightforward application of well-established laboratory-based chemical analysis techniques to this national problem. Beyond any solution to this immediate problem also lies a present and long-term need to monitor low-level subsurface contaminations associated with such storage facilities. While an approach to removing high-level nuclear wastes has been identified (vitrification), the chemical analysis technology available in-hand to assist in this important task is inadequate.

The general aim of the work embodied in this research project is to design and implement a new sensor technology which offers the unprecedented levels of specificity needed for analysis of the complex chemical mixtures found at USDOE sites nationwide. The new sensor concept combines the elements of electrochemistry, spectroscopy and selective partitioning into a single device that provides three levels of selectivity.

This type of sensor has many potential applications at DOE sites. As an example, the enhanced specificity embodied in this new sensor design is well-suited to the analytical problem posed by the addition of ferrocyanide to radioactive tank wastes at the USDOE Hanford Site. Various radioactive wastes from defense operations have accumulated at the Hanford Site in underground waste tanks since the early 1940s. During the 1950s, additional tank storage space was required to support the defense mission. Hanford Site scientists developed two procedures to obtain this additional storage volume within a short time period without constructing additional storage tanks. One procedure involved the use of evaporators to concentrate the waste by removing water. The second procedure involved developing precipitation processes for scavenging radio-cesium and other soluble radionuclides from tank waste liquids. The scavenging processes used sodium and potassium ferrocyanide and nickel sulfate to precipitate radioactive cesium from solutions containing nitrates and nitrites. Radioactive strontium and cobalt were scavenged from some of the solutions using calcium or strontium nitrate and sodium sulfide, respectively. After allowing the radioactive precipitates to settle, the decontaminated solutions were pumped to disposal cribs, thereby providing additional tank storage volume. Later, some of the tanks were found to be leaking; pumpable liquids were removed from these tanks, leaving behind a wet solid (sludge) residue containing the ferrocyanide precipitates. In implementing this process, approximately 140 metric tons of ferrocyanide, [calculated as $Fe(CN)_6{}^{4}$], were added to waste that was later routed to 18 large (750,000 to 1,000,000 gallon) underground single shell tanks (SSTs). Since ferrocyanide/nitrate mixtures are potentially explosive in the dry state at elevated temperatures, a ferrocyanide remote sensor is needed for characterization of tank waste before and during the disposal process.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§+ RL-TW04	C-169	Retrieval Project
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
§ SR-HL05	C-265	Vitrification
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
NV214	C-53	Industrial Sites
+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER06	C-141	Decontamination and Decommissioning
RL-TP10	C-163	Accelerated Deactivation
RF014	C-213	Industrial Zone Closure Project
+ SR-SW01	C-281	Consolidated Incinerator Facility

Environmental Management Science Program Research in Ohio

University of Cincinnati

60474-OH - Develop and Demonstrate Novel Ultrahigh Sensitivity Heavy Noble Gas Detectors for Long-Term Monitoring of Spent Fuel and TRU Waste

Year of Award: 1997 **Amount of Award:** $608,760
Problem Area: Health / Ecology / Risk
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Sensors and Techniques
Principal Investigator: Dr. John D. Valentine, 513-556-2482, John.Valentine@UC.Edu
Major Collaborator(s): Kenny Gross at Argonne National Laboratory
For More Information: http://www.doe.gov/em52/60474.html

Description Provided by Investigator:

A University of Cincinnati/Argonne National Laboratory (UC/ANL) team will develop and demonstrate novel ultrahigh sensitivity heavy noble gas (krypton, xenon, and radon) detectors for long-term monitoring of spent fuel and TRU waste, as well as for distinguishing background radon alpha particles from other alpha emissions in air monitors. A new technique for concentrating the heavy noble gases from air will be integrated with state-of-the-art radiation detector technology to provide sensitivities on the order of two orders of magnitude better than current technology. In addition, these detectors can be configured such that heavy noble gas concentration in air is monitored continuously and recorded in real-time and in situ. This real-time data acquisition coupled with the ability to measure the beta particles and gamma rays emitted by krypton and xenon in coincidence mode will result in an enhanced ability both to use spectral information to detect and identify the different noble gas isotopes and to discriminate against all other signals. Finally, such an integrated concentration and detection system has the potential to provide low-cost and low-complexity detectors which would be ideally suited for long-term monitoring and fieldable air monitors.

It is proposed that a broad range of potential detectors and measurement techniques be identified and evaluated for use in DOE Environmental Management applications. Furthermore, at least two of the most promising techniques for detecting the heavy noble gas emissions will be developed experimentally. First, the concentrated radioactive gases can be mixed directly with standard proportional detector filled gases such that a 100% detection efficiency is realized when the mixture is passed through a proportional detector. Second, the concentrated gases can be used in scintillator flow-cell geometry to achieve a similar detection efficiency. While both of these techniques provide the ability to distinguish alpha and beta particle interactions within the detector, a gamma-ray spectroscopy detector can be used in coincidence mode with both techniques to further enhance background discrimination and species identification. Consequently, coincidence mode operation will also be demonstrated experimentally using both the proportional and the flow-cell detectors. If additional detectors and techniques are identified as promising, similar experimental development will be pursued for those systems. Finally, the developed detection systems will be evaluated and one or more systems identified, constructed, and demonstrated. This final demonstration of the technology will be conducted initially in the laboratory environment to establish operating characteristics, and subsequently will be conducted at a DOE EM site. To complete this detector development, a three-year team effort is proposed.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Health / Ecology / Risk problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Health / Ecology / Risk".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
NV212	C-49	Underground Test Area (UGTA)
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
RL-ER08	C-147	Groundwater Management
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Oklahoma

University of Oklahoma

60041-OK - Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration

Year of Award: 1997 **Amount of Award:** $538,997
Problem Area: Decontamination and Decommissioning
Science Category/SubCategory: Separations Chemistry / Ligand Design and Ion-exchange
Principal Investigator: Dr. John F. Scamehorn, 405-325-5811, scamehor@mailhost.ecn.ou.edu
Major Collaborator(s): Dr. Cynthia E. Palmer at Lawrence Livermore National Laboratory
For More Information: http://www.doe.gov/em52/60041.html

Description Provided by Investigator:

The research program is a joint project between the University of Oklahoma Institute for Applied Surfactant Research and the Lawrence Livermore National Laboratory. The project involves use of an innovative class of separation techniques developed at the University of Oklahoma over the past 15 years and the expertise of Lawrence Livermore National Laboratory in the study of highly toxic radioisotopes such as plutonium and the experimental capability to handle these materials. This unique collaboration will permit a comprehensive study of the use of colloid-enhanced ultrafiltration processes to remove and recover important radionuclide ions and associated contaminants from aqueous streams. The removal of the following radioactive elements from water will be investigated: plutonium, thorium, strontium, and uranium. Pollutant ions which are present as a result of previous treatment or processing of the radionuclide ions whose removal will be studies here include lead and chromate; therefore, this research will apply mixed waste problems. A postdoctoral associate will link the two research groups together by spending a fraction of the year at the University while studying plutonium removal at Livermore the rest of the time.

The colloid-enhanced ultrafiltration methods all involve the addition of water-soluble components such as polyelectrolytes and ligands to bind target ions. In many cases, a high degree of selectivity can be attained by using a ligand which specifically complexes the target ion and is then attached to a colloid such as polyelectrolyte. For example, in this work, plutonium, thorium, strontium, uranium, and lead can all be removed in a highly selective fashion with available ligands or those which we will synthesize as part of this project. Subsequent ultrafiltration produces purified water and a homogeneous aqueous solution containing the concentrated pollutants and added colloid. Since only liquid phases are present, these techniques can be operated at steady state and are intrinsically low-energy processes. Downstream methods to separate the pollutants from the colloids and ligands concentrate the contaminants (waste minimization) for disposal and permit recycle of the colloid for reuse. These methods have been demonstrated in general in the laboratory and in field tests on actual groundwater and will be developed for the specific target ions to be studied in this investigation.

An advantage of the colloid-enhanced ultrafiltration processes to be used here is that toxic cations and anions can be simultaneously removed from the water. As an example, a cationic polyelectrolyte can be chosen to bind multivalent anions (e.g., chromate or CrO_4^{2-}) while anionic ligands which selectively bind target cations (e.g., thorium or Th^{4+}) are themselves electrostatically bound to the polyelectrolyte. The result is removal of multivalent anionic and selective removal of cationic pollutants in a single step. After concentration of the colloids and target ions into a retentate stream by ultrafiltration, the polyelectrolyte and ligand can be regenerated by adjustment of pH and electrolyte concentration. This project would involve determination of this mixed ion removal process efficiency and optimum operating conditions for the systems of interest (e.g., selection of polyelectrolyte and ligand, highest concentration of colloid attainable during actual ultrafiltration).

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Decontamination and Decommissioning problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Decontamination and Decommissioning".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
§ OR-43204	C-77	ORNL Bethel Valley Deactivation and Decommissioning
§ OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
§+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
§+ RL-ER06	C-141	Decontamination and Decommissioning
§+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
+ OR-46301	C-107	Portsmouth Remedial Action
RL-ER08	C-147	Groundwater Management
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in Oregon

Oregon State University

55196-OR - In Situ, Field Scale Evaluation of Surfactant Enhanced DNAPL Recovery Using a Single-Well, Push-Pull Test

Year of Award: 1996 **Amount of Award:** $616,560
Problem Area: Remedial Action
Science Category/SubCategory: Hydrogeology / Dense Non-Aqueous Phase Liquid (DNAPL) Dynamics
Principal Investigator: Dr. Jonathan D. Istok, 541-737-6838, istokj@cyclops.ce.orst.edu
Major Collaborator(s): Jennifer A. Field at Oregon State University
For More Information: http://www.doe.gov/em52/55196.html

Description Provided by Investigator:

Surfactant enhanced DNAPL recovery involves the use of injected surfactants to increase the solubility and/or mobility of DNAPL in the subsurface to reduce the time and cost required for site remediation. The successful design of a surfactant enhanced DNAPL recovery system requires a quantitative understanding of the competing processes of DNAPL solubilization and mobilization, and sorption, precipitation, and microbial degradation of injected surfactant components. **An innovative new site-characterization technology, the single-well, "push-pull" test method**, is currently under development at Oregon State University and has been successfully used in the field to determine a wide range of aquifer physical, chemical, and biological characteristics. A push-pull test consists of the controlled injection of a prepared test solution into a single monitoring well followed by the extraction of the test solution/groundwater mixture from the same well. The type, combination, and concentration of injected solutes is selected to investigate specific aquifer characteristics.

The overall goal of this project is to further develop the single-well, "push-pull" test method as a new site characterization and feasibility assessment tool for studying the fundamental fate and transport behavior of injected surfactants and their ability to solubilize and mobilize DNAPLs in the subsurface. The specific objectives are:

(1) to develop a modified "push-pull" test for use in identifying and quantifying the effects of sorption, precipitation, and biodegradation on the fate and transport of injected surfactants,

(2) to use the developed test method to quantify the effects of these processes on the ability of injected surfactants to solubilize and mobilize residual phase trichloroethylene, and

(3) to demonstrate the utility of the developed test method for performing site characterization and feasibility studies for surfactant enhanced DNAPL recovery systems.

The project is a **collaborative research effort** between the Departments of Civil Engineering and Agricultural Chemistry at Oregon State University (OSU). The project is interdisciplinary and it is designed to utilize the scientific skills, experimental systems, and analytical capabilities available in each department. To address the three objectives, the research plan combines **controlled intermediate-scale laboratory experiments in unique physical aquifer models** with a parallel series of **pilot-scale field experiments** in existing monitoring wells at selected trichloroethylene (TCE) contaminated field sites. The physical models areconstructed in the shape of a circular arc ('piece of pie') to represent the alternating diverging/converging radial flow field near a well during the injection and extraction phases of a push-pull test. Intermediate-scale experiments (as opposed to studies in small scale batch reactors or columns) were selected for this project because they can provide **spatial and temporal information** on surfactant sorption, precipitation, and biodegradation in the vicinity of the monitoring well during a field push-pull test, they can quantify the effects of these processes on surfactant composition, concentration, and activity, and because they allow the calculation of **accurate mass balances** for all solutes in both aqueous and solid phases. To address Ojectives 1 and 2, laboratory push-pull tests in the physical aquifer models will be conducted using **native aquifer sediment and groundwater** collected from uncontaminated portions of a TCE contaminated field site located in Corvallis, Oregon near OSU; an identical series of field push-pull tests will be performed at the same site using existing monitoring wells located in an uncontaminated portion of the aquifer and in locations where the presence of residual TCE liquid has been confirmed by soil coring and free product recovery. To address

Objective 3, additional field push-pull tests will be conducted at selected DOE sites including the Building 834 Operable Unit at Lawrence Livermore National Laboratory Site 300, and at additional sites at Pacific Northwest National Laboratories and Sandia National Laboratories.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ OR-46301	C-107	Portsmouth Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Oregon

Oregon State University

60158-OR - Development of Radon-222 as a Natural Tracer for Monitoring the Remediation of NAPL Contamination in the Subsurface

Year of Award: 1997 **Amount of Award:** $403,886
Problem Area: Remedial Action
Science Category/SubCategory: Hydrogeology / Dense Non-Aqueous Phase Liquid (DNAPL) Dynamics
Principal Investigator: Dr. Lewis Semprini, 541-737-6895, semprinl@ccmail.orst.edu
For More Information: http://www.doe.gov/em52/60158.html

Description Provided by Investigator:

One of the major obstacles preventing cost-effective cleanup of many DOE sites is the current inability to accurately locate and quantify residual nonaqueous phase liquid (NAPL) contamination. The recently developed *natural radon tracer method* has the potential to provide a rapid, low-cost, nondestructive, and noninvasive method for routine use in quantifying residual NAPL in the subsurface. The method is based on detecting changes in radon concentration in groundwater samples collected from existing monitoring wells. In the subsurface, radon-222 (radon) is produced by the decay of naturally occurring radium-226 contained in the mineral fraction of aquifer solids. In groundwater radon occurs as a dissolved gas, with a half-life of 3.83 days. In the absence of NAPL, radon concentrations quickly reach a maximum value that is determined by the mineral composition of the aquifer solids, which controls the rate of radon emanation. In the presence of NAPL, however, radon concentrations are substantially reduced due to the preferential partitioning of radon into the organic NAPL phase. Moreover, the reduction in radon concentration is quantitatively correlated with residual NAPL saturation. **Thus, by measuring radon concentrations in a number of wells it is possible to identify those locations where NAPL is likely present and to quantify residual NAPL saturation in each location.**

In an exploratory grant funded by the DOE through the Western Region Hazardous Substance Center of the EPA, the feasibility of the radon method was demonstrated by Dr. Semprini using a combination of laboratory studies and numerical modeling. The method has also been successfully used to detect residual NAPL in a controlled release experiment and to identify possible NAPL locations at a DOE field site. The research will focus on the fundamental processes governing radon emanation, partitioning, and transport in heterogeneous subsurface environments and the use of the method to identify and quantify residual NAPL saturations at a DOE site undergoing active remediation to remove NAPL.

The specific research objectives are:

1. to determine the dependence of radon emanation from natural aquifer solids on the composition and properties of fluids filling the pore space,
2. to determine radon NAPL: water partition coefficients for a broad range of LNAPLs and DNAPLS of environmental concern,
3. to quantify relations between radon emanation and partitioning and regional flow and transport in heterogeneous subsurface materials before and during NAPL remediation.
4. to test the feasibility of the radon method to identify and quantify residual NAPL during site remediation, and
5. to conduct numerical simulations to extend the applicability of laboratory and field results to a wider range of DOE sites.

The research combines **small-scale laboratory studies, intermediate-scale laboratory studies in unique physical aquifer models, field studies** at a DOE site undergoing active NAPL remediation, and **numerical simulations** to extend the range of applicability of the laboratory and field results to a wider range of NAPL contamination problems at DOE sites.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

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Project ID	Page #	Project Title
§ NV214	C-53	Industrial Sites
§ RF014	C-213	Industrial Zone Closure Project
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning

Environmental Management Science Program Research in Pennsylvania

Pennsylvania State University

54122-PA - A Broad Spectrum Catalytic System for Removal of Toxic Organics from Water By Deep Oxidation

Year of Award: 1996 **Amount of Award:** $327,000
Problem Area: Remedial Action
Science Category/SubCategory: Separations Chemistry / Catalyst Chemistry and Waste Treatment
Principal Investigator: Dr. Ayusman Sen, 814-863-2460, asen@chem.psu.edu
For More Information: http://www.doe.gov/em52/54122.html

Description Provided by Investigator:

Toxic organics in water constitute a very serious and persistent environmental hazard. Many are difficult to remove efficiently either through bioremediation or by presently known catalytic systems. It has been found that metallic palladium affects the removal of toxic organics and polymers by catalyzing their deep oxidation by dioxygen in aqueous medium at about 80-90°C, in the presence of carbon monoxide. This system possesses several attractive features not found simultaneously in other reported systems. These are (a) the ability to directly utilize dioxygen as the oxidant, (b) the ability to carry out the deep oxidation of a particularly wide rage of functional organics, and (c) the ease of recovery of the catalyst by simple filtration. A comprehensive study of this catalytic system is proposed. The research will encompass (a) the elucidation of the detailed mechanism of oxidation, including the identification of the active species and the nature of the bond-breaking and oxidation steps, and (b) the identification of the classes of organics, including functionalized (especially, mono and perhalogenated) aromatics and aliphatics, organonitrogen, organophosphorus, organoarsenic, and organosulphur compounds, as well as polymers, that can be efficiently oxidized and thereby removed from water. In addition, the possibility of designing more efficient hybrid catalytic oxidation systems will be examined. The ultimate goal of the research is the design of one or more cleanup systems that would be useful from a practical standpoint. If successful, the research should lead to mild, efficient, procedures for emission-free destruction of a wide range of harmful organics, as well as simultaneous water purification. While the design of a procedure for removal of organics and polymers from water would be the first priority of research, the use of the same catalyst system for the deep oxidation of non-aqueous phase organics in either a mixed solvent system or in a two-phase (water/liquid organic substrate) system will also be investigated.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV214	C-53	Industrial Sites
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ OR-46301	C-107	Portsmouth Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER02	C-129	200 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ RF014	C-213	Industrial Zone Closure Project
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
ID-HLW-101	C-29	High-Level Waste Pretreatment
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW05	C-173	Process Waste Support
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
+ SR-HL01	C-249	H-Tank Farm
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
SR-HL05	C-265	Vitrification
+ SR-SW01	C-281	Consolidated Incinerator Facility
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in Pennsylvania

Pennsylvania State University

55171-PA - Development of Advanced In-Situ Techniques for Chemistry Monitoring and Corrosion Mitigation in SCWO Environments

Year of Award: 1996 **Amount of Award:** $696,395
Problem Area: Mixed Waste
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Sensors and Techniques
Principal Investigator: Dr. Digby D. Macdonald, 814-863-7772, ddm2@psuvm.psu.edu
Major Collaborator(s): Dr. Karen M. Garcia at Idaho National Engineering and Environmental Laboratory
For More Information: http://www.doe.gov/em52/55171.html

Description Provided by Investigator:

We propose to develop chemical and corrosion sensors for use in high subcritical and supercritical aqueous environments, to improve their precision and reliability, and to use them to characterize the fundamental properties of supercritical aqueous solutions. A better understanding of phenomena in supercritical water will enable us to develop advanced, safe, and emission-free waste treatment processes for the destruction of DOE waste. The work will emphasize the development of advanced reference electrodes, fabrication of pH sensors and redox sensors, as well as exploring electrochemical emission spectroscopy as a means of characterizing metal/water interactions (including corrosion). We will also define a practical pH scale for use with supercritical aqueous systems. This work will be carried out in cooperations with Idaho National Engineering Laboratory (INEL), and it will employ the bench scale reactor at INEL to test the sensors, and to perform studies of aqueous chemistry and electrochemistry at supercritical temperatures in model waste streams.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW03	C-287	Mixed Low Level Waste Project
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-TW04	C-169	Retrieval Project
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RF014	C-213	Industrial Zone Closure Project
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Pennsylvania

Pennsylvania State University

60017-PA - Removal of Technetium, Carbon Tetrachloride, and Metals from DOE Properties

Year of Award: 1997 **Amount of Award:** $390,000
Problem Area: High Level Waste
Science Category/SubCategory: Separations Chemistry / Technetium Chemistry and Separations
Principal Investigator: Dr. Thomas E. Mallouk, 814-863-9637, tom@chem.psu.edu
Major Collaborator(s): Dr. John G. Darab at Pacific Northwest National Laboratory
For More Information: http://www.doe.gov/em52/60017.html

Description Provided by Investigator:

This research is a three year project involving close collaboration between chemists at Pennsylvania State University and materials scientists at Pacific Northwest National Laboratory (PNNL). The goal of the project is the development and characterization of supported reducing agents, and solid waste forms derived from them, which will be effective in remediation of aqueous wastes.

The work follows the recent discovery that zero-valent metals, such as iron, are effective decontaminants for waste streams containing chlorinated hydrocarbons. Preliminary data, obtained at Penn State and elsewhere, have shown that the same strategy will be effective in reducing soluble compounds containing toxic metals (technetium, lead, mercury, and chromium) to insoluble forms. The Penn State group has prepared a new class of powerful reducing agents, called Ferragels, which consist of finely divided zero-valent metals on high surface area supports. Because the rate of the surface oxidation-reduction reaction depends on available surface area, Ferragels are more effective in every case tested to date than unsupported metals. The project will further develop and investigate the application of these composite materials to problems relevant to the DOE-EM mission, namely the detoxification of waste streams containing technetium, carbon tetrachloride, and toxic metal ions. The Penn State group will work closely with the PNNL group to prepare materials that are compatible with the highly corrosive liquid fraction of Hanford site tank waste, to conduct tests with waste simulants containing technetium, and to formulate and characterize vitrified waste forms derived from these materials.

Technetium (Tc) removal is a high priority need for the Hanford tank system. The proposed waste separation, pretreatment, and vitrification processes for this waste involve separation into solid high level waste (HLW) and liquid low level waste (LLW) fractions. The latter will contain most of the Tc, predominantly in the +7 oxidation state as the pertechnetate ion (TcO_4^-). Vitrification of these wastes is very problematic because Tc^{7+} compounds are volatile at high temperatures, and the presence of large quantities of nitrate and nitrate in the LLW ensures that the melts remain oxidizing. Methods of extracting Tc from the LLW prior to concentration and vitrification are urgently needed, in order to address this volatility problem, as well as to reduce the total volume of vitrified waste. These needs are driven by both safety and cost considerations. Tests conducted at Penn State, using ReO_4^- (as a non-radioactive surrogate for TcO_4^-) show that it is quantitatively reduced to an insoluble, non-volatile Re4+ compound by iron-on-silica Ferragel. In parallel experiments, the PNNL group has established that the vitrification chemistry of ReO_4^- is very similar to that of TcO_4^-. Problems remain with the instability of the silica support under the highly alkaline conditions of simulated tank waste, and the oxidation of iron in Ferragel by nitrite. The research includes the synthesis of Ferragels with base-insoluble supports (TiO_2, ZrO_2, SnO_2) that will be compatible with vitrification or glass-ceramic encapsulation. Some of these supports are feedstocks for low-melting glass compositions recently developed by the PNNL group. PNNL will study the vitrification chemistry of Ferragels, and will determine the oxidation state and coordination environment of Re and Tc in vitrified waste forms, using X-ray absorption spectroscopies. Surface chemical modification strategies are proposed that will cause ReO_4^- and TcO_4^- ions to partition into the surface layer selectively, thereby minimizing the corrosion of iron by nitrite in the tank waste simulant. These surface modification experiments will be accompanied by detailed kinetics and materials characterization studies, carried out at Penn State. Similar synthetic and analytical strategies will be applied to remediation of aqueous wastes containing halogenated organics, specifically CCl4, and soluble metal ions, such as mercury, lead, and chromium, which have been identified as medium-priority needs of the Environmental Management Science Program.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
§ SR-HL05	C-265	Vitrification
AL024	C-3	Grand Junction Office (GJO) All Other Projects
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-48101	C-99	Offsite Remedial Action
+ OR-45301	C-103	Paducah Remedial Action
RL-ER08	C-147	Groundwater Management
RF014	C-213	Industrial Zone Closure Project
+ SR-ER06	C-227	Upper Three Runs Project
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in Pennsylvania

Pennsylvania State University

60219-PA - Development of Advanced Electrochemical Emission Spectroscopy for Monitoring Corrosion in Simulated DOE Liquid Waste

Year of Award: 1997 **Amount of Award:** $350,000
Problem Area: High Level Waste
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Sensors and Techniques
Principal Investigator: Dr. Digby D. MacDonald, 814-863-7772, ddm2@psuvm.psu.edu
Major Collaborator(s): Dr. George R. Engelhardt at Pennsylvania State University
For More Information: http://www.doe.gov/em52/60219.html

Description Provided by Investigator:

The Department of Energy currently stores millions of gallons of high level liquid radioactive waste in underground, carbon steel-lined concrete tanks at the Hanford Reservation in the state of Washington and at the Savannah River Site in South Carolina. Because of the indefinite time of storage, general corrosion, even though it may occur only at a low rate, must be considered as a principal threat to tank integrity. However, various forms of localized corrosion (pitting, crevice corrosion, and stress corrosion cracking) are known to occur on iron and carbon steel in alkaline environments, in general, and on carbon steel in DOE liquid waste environments, in particular. Because localized corrosion often results in sudden and unexpected failures, knowledge of the conditions under which localized corrosion occurs is vital for assessing the possibility of failure and for assessing remaining life.

In this program, we propose to use a variety of electrochemical techniques, but most notably Electrochemical Emission Spectroscopy (EES), to explore the fundamental aspects of the general and localized corrosion behaviors of iron and carbon steel in alkaline environments, including stimulated DOE liquid waste. Our goal is to resolve important mechanistic issues using the most modern electrochemical and analytical techniques. These include the analysis of EES data in terms of non-linear dynamics methods; the use of Electrochemical Impedance Spectroscopy (EIS), rotating ring-disk voltammetry, chronoamperometry, and steady-state (dc) polarization techniques to explore the passive state of iron in these media; the determination of passivity breakdown potentials and induction times, as well as the characterization of electrochemical emissions due to metastable pitting; the analysis of electrochemical noise in the coupling current between a crack or a crevice and the external surfaces as a means of determining the mechanisms of these processes; and the further development of deterministic theories and models for predicting the evolution of corrosion damage. These studies are expected to resolve important mechanistic issues, including the origin of electrochemical emissions in general corrosion, the viability of current deterministic models and theories for describing the passive state and for predicting passivity breakdown and the nucleation of pitting, and the delineation of anodic dissolution and hydrogen-induced fracture as the mechanism of crack propagation in carbon steels in highly alkaline solutions. Although the principal emphasis will be on the fundamental aspects of the subject, we will also assess the potential of techniques developed in this work to be used for in-situ, continuous monitoring of corrosion in DOE's storage tanks.

The proposed, three-year research program will be carried out in The Pennsylvania State University's Center for Advanced Materials (CAM) under the direction of Prof. Digby D. MacDonald and Dr. George Engelhardt. Researchers in CAM have extensive experience in studying electrochemical and corrosion phenomena on metals and alloys under extreme environmental conditions, and many of the techniques developed in this previous work will be employed in the research program.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§+ RL-TW04	C-169	Retrieval Project
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
§ SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Pennsylvania

University of Pennsylvania

54856-PA - Structural Biology of the Sequestration & Transport of Heavy Metal Toxins: NMR Structure Determination of Proteins Containing the -Cys-X-Y-Cys-metal Binding Motifs

Year of Award: 1996 **Amount of Award:** $980,000
Problem Area: Health / Ecology / Risk
Science Category/SubCategory: Health Science / Molecular, Structural and Genomic Science
Principal Investigator: Dr. Stanley J. Opella, 215-898-6459, opella@chestnut.chem.upenn.edu
For More Information: http://www.doe.gov/em52/54856.html

Description Provided by Investigator:

There are enormous amounts of heavy metals in the environment, much of it in the form of organometallic compounds resulting from various types of industrial and military waste. Nearly all of these metals and compounds are highly toxic to biological organisms including humans. However, some bacteria thrive in the presence of high concentrations of heavy metal toxins because they possess efficient mechanisms for the detoxification of these metals and compounds. Heavy metals appear to be universally toxic because of their non-selective chemistry, for example Hg(II) reacts with essentially all exposed sulfhydryl groups on proteins, thus, it may seem surprising that any organism at all can survive these chemical insults much less those that grow in a toxic milieu. However, the prebiotic environment was undoubtedly heavily polluted with heavy metals from geological processes, and the most primitive organisms simply had to evolve mechanisms for dealing with them if they were going to be able to utilize Cys, His, and the other amino acids that contribute to metal binding sites in their proteins. Genes associated with bacterial resistance to Ag, AsO_2, AsO_4, Bi, Cd, Co, CrO_4, Cu, Hg, iNi, TeO_3, TI, Pb, Zn, and other metals of environmental concern have been described (Silver, 1992; Silver and Walderhaug, 1995).

The research is based on the premise that the proteins encoded in these genes are an untapped source of reagents as well as chemical strategies for removal of heavy metal toxins from the environment. Our approach is to apply the methods of structural biology, which have previously been used primarily in biomedical applications, to bioremediation. The first and most essential step is to determine the structures of the proteins involved in binding and transport of heavy metals.

In addition to biological toxicity through damage to proteins, heavy metals are directly involved in several human diseases where transport functions have gone awry. Both Menkes and Wilson diseases are associated with improper copper metabolism, and the genes responsible for these diseases have been shown to correspond to P-type ATPases (Lutsenko and Kaplan, 1995). These large proteins have multiple repeats of a metal binding domain that is highly homologous to one found in bacterial systems. Indeed, mutations in this region of the proteins results in human diseases (Chelly et al., 1993; Mercer et al. 1993). Further, a possible connection has been found between the mercury in dental amalgam fillings and antibiotic resistance of bacteria that cause human infectious diseases (Summers et al. 1993). The genes that protect the bacteria against mercury are on a plasmid along with those for antibiotic resistance, and oral and intestinal bacteria have been found to have increased resistance to both mercury and antibiotics following the placement of dental fillings. Since small amounts of mercury are constantly released from dental fillings, the selection of mercury resistant bacteria possessing genes for the detoxification system may contribute to medically important antibiotic resistance in humans.

We propose to gain insight into biological detoxification and the possibilities for protein based ex vivo bioremediation of heavy metals by determining the structures of several bacterial and human proteins that contain metal binding modules that utilize the -Cys-X-Y-Cys-motif. These proteins are as diverse as the 8 kD periplasmic mercury binding portein merP of the bacterial mercury detoxification system (Summers, 1986) and the 200 kD human heavy-metal-transporting P-type ATPases (Lutsenko and Kaplan, 1995) which contain up to six metal binding modules homologous to merP. This research is a direct outgrowth of our initial structural studies of two of the proteins of the bacterial mercury detoxification system, merP (periplasm) and merT (transport). Itrepresents a significant extension to other proteins that share the common metal binding motif, but are used in different contexts and detoxify other metals. This research has the potential to substantially enhance the possibilities for the development of protein based bioremediation of heavy metal toxins. It is highly feasible because of the extensive preliminary results obtained on merP and merT.

The immediate focus of our research is on the structural biology of proteins responsible for the binding and transporting of metals across across membranes. Once the structures of these proteins are determined, it should be possible to re-engineer them using both site directed and random mutagensis methods to optimize their functions, alter their metal binding specificities, and stabilize their structures. It may then be feasible to place the altered proteins in natural or synthetic membranes to make biologically based devices for the detection and separation of mercury or other metals. It may also be feasible to place the genes for these altered, optimized proteins in plants, which will effect removal of the heavy metal toxins from the environment (Rugh et. al., 1996). Although such long-term practical benefits from the proposed basic research are speculative at this early stage of the program, it is important to keep in mind the broad environmental implications of what can be done with the structural information obtained from the research throughout the program period.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Health / Ecology / Risk problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Health / Ecology / Risk".

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Project ID	Page #	Project Title
AL024	C-3	Grand Junction Office (GJO) All Other Projects
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ OR-48101	C-99	Offsite Remedial Action
+ OR-45301	C-103	Paducah Remedial Action
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
RL-ER08	C-147	Groundwater Management
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project
SR-HL05	C-265	Vitrification
+ SR-SW01	C-281	Consolidated Incinerator Facility
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in South Carolina

Savannah River Ecology Laboratory

55410-SC - Determining Significant Endpoints for Ecological Risk Analyses

Year of Award: 1996 **Amount of Award:** $897,666
Problem Area: Health / Ecology / Risk
Science Category/SubCategory: Health Science / Risk Assessment
Principal Investigator: Dr. Thomas G. Hinton, 803-557-7454, thinton@srel.edu
Major Collaborator(s): F. Ward Whicker at Colorado State University
For More Information: http://www.doe.gov/em52/55410.html

Description Provided by Investigator:

Risk analyses, both human health and ecological, will be important factors in determining which DOE sites should be cleaned up and in deciding if acceptable performance standards have been met. Risk analysis procedures for humans use the individual as the 'unit' of observation, and the individual's health as the risk assessment endpoint, typically measured in terms of lifetime cancer risk. For ecological risk assessments, however, the proper endpoint is much debated because the appropriate unit of interest for nonhumans may not be individuals; risk might be assessed more properly at higher levels of biological organization, such as the population, community or ecosystem. Seldom is there concern over an individual fish or tree, but rather that the fish and tree populations remain viable.

Contaminants can affect all levels of biological organization, from individual cells to ecosystems. Recent technology has made it relatively easy to measure cellular and molecular abnormalities; thus, much ecotoxicological research concentrates on effects at these lower levels of organization. Documenting effects at levels of the individual, population, or community is more complex and difficult (Forbes and Forbes, 1994, Calow and Sibly, 1990). Therefore, a disparity exists in most ecological risk analyses between what generally is measured and what needs to be measured if the population is the ultimate unit of interest and ecological relevance.

THE PROBLEM

Molecular damage generally represents a sublethal endpoint that may provide early warning of potential contaminant impact, but the consequences of molecular damage to higher levels of biological organization have not been well documented (Clements and Kiffney, 1994; Underwood and Peterson, 1988; Forbes and Calow, 1996). Environmental risk analyses that use molecular effects as endpoints are of unknown value because of the uncertainities in quantifying the significance to individuals, populations and communities.

The problem of defining a proper endpoint for ecological risk analyses has wide-reaching implications. Inherent in any assessment of risk are the criteria used in determining what is a 'significant risk'. Determining significance is particularly difficult at contaminated environments where low-level exposures may produce subtle responses in organisms (Forbes and Calow, 1996). Low-level exposures to radionuclides and other contaminants occur on many DOE sites. The ultra-sensitivity of modern genetic techniques might allow investigators to document molecular damage in organisms from DOE sites with very low contaminant levels. However, if such molecular damage has little long-term impact on the physiology of the individual or the dynamics of the population, do these sites actually pose significant environmental risks? Do they require multimillion dollar cleanup operations? Baker et al. (1996) report a mutation rate in the mitochondrial DNA of voles collected from Chernobyl, Ukraine, that is hundreds of times greater than expected, even though the voles appear to be thriving. Thus, nonhuman risk analyses based on molecular damage without an understanding of the impacts to higher levels of biological organization, could cause cleanup strategies on DOE sites to be overly conservative and unnecessarily expensive.

In essence, a population level dose-response curve is needed for nonhuman species. However, a meaningful dose-response curve is plagued by uncertainties on both axes; the relevant ecological endpoint used for the response is much debated, and the errors associated with the dose are often too large for meaningful data interpretation. In other words, how can dose to free ranging organisms be quantified, and what are the appropriate response variables?

For chronic, low-level radioactive contamination accurate dosimetry is problematic. Chromosomal aberrations have been recognized for many years as perhaps the most important form of radiation damage. But the kinds of aberrations that have been readily visible by microscopic observation eventually kill the cells that bear them (Muller, 1927). Such aberrations appear in the first post-irradiation mitosis, and have been used fairly extensively as 'biological dosimeters'. Because cells containing these aberrations die, their frequencies in succeeding cell generations rapidly decrease. The drawback of most current techniques is that the 'biological dosimeter' does not indicate cumulative damage, and it is necessary to sample cells from individuals soon after exposure in order to obtain a sensitive and reliable estimate of dose. Once a method is found that accurately estimates dose, then relevant response variables still must be chosen that are in some way related to population 'health'.

THE SOLUTION

Research is needed to better determine the ecological risks and associated uncertainties from toxic and radioactive contaminants. More precisely, research is needed to determine the relevancy of varied levels of sublethal cellular damage to the performance of individuals and characteristics of populations exposed to chronic, low-level radiation, as is typically found on many DOE sites.

Significant Endpoints

We believe the ecological relevance of low-level exposures can be elucidated by using metabolic rate (MR) as an indicator of contaminant stress. Metabolic rates of individuals may well be the best physiological measure of sublethal stress as it reflects multiple processes occuring within an organism, and at the same time has direct relevance to other processes occurring at the individual and population levels. Metabolic rate is a measure of the energetic efficiency of the organism, and thus should reflect significant energetic 'costs' to stressed organisms with implications for such processes as energy storage, growth and reproduction (Forbes and Calow, 1996). Organisms acquire and assimilate a finite amount of energy from the resources within their environment. Energy must be allocated to the basic physiological processes necessary for survival (maintenance costs), and then the remainder can be partitioned to growth, fat storage and reproduction (Congdon et al., 1982; Congdon, 1989). Exposure to contaminants generally elicits some kind of physiological or behavorial response from the organism that requires reallocating a portion of the organism's assimilated energy. Thus, each response has an associated cost, subtracting from the energy resources that the organism would otherwise use for maintaining and propagating life. Responses to toxic stress can be considered trade-offs among maintenance, storage, growth rate and reproductive output (Sibly and Calow, 1989; Krebs and Loeschcke, 1994). Trade-offs may be quite subtle, yet still impact populations. One of the principal questions is how relevant are the subtle responses, and at what point are population effects observable?

Responses of organisms to contaminants can be grouped into several general categories (Forbes and Calow, 1996):

> "avoidance or escape reactions; exclusion (for example, many aquatic animals exposed to toxic chemicals secrete mucus onto exposed surfaces); removal (incoming toxicants might be actively pumped out); detoxification, possibly followed by excretion (e.g. by sequestration in granules or viametabolic transformation); and repair of damage caused by toxicants."

A general model predicts a positive relationship between metabolic rate and either exposure duration or concentration of contaminants, until stress is severe enough that metabolism itself is impaired (Basha et al., 1984; LeBras, 1987; Calow, 1989). We think that changes in metabolic rate can be a criterion for determining whether effects observed following contaminant exposure are relevant to higher levels of biological organization. If costs are not detected at the individual level (i.e. an increased MR) then demonstrating implications for population and community-level processes becomes extremely difficult.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Health / Ecology / Risk problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Health / Ecology / Risk".

Environmental Management Science Program Research in South Carolina

Savannah River Technology Center

60401-SC - Mechanism of Pitting Corrosion Prevention by Nitrite in Carbon Steel Exposed to Dilute Salt Solutions

Year of Award: 1997 **Amount of Award:** $650,000
Problem Area: High Level Waste
Science Category/SubCategory: Materials Science / Surface Chemistry
Principal Investigator: Dr. Philip E. Zapp, 803-725-2567, Philip.Zapp@srs.gov
Major Collaborator(s): Dr. John Van Zee at the University of South Carolina
For More Information: http://www.doe.gov/em52/60401.html

Description Provided by Investigator:

The overall goal of this project is to develop a fundamental understanding of the role of nitrite in preventing the breakdown of protective oxide coating on steel and the onset of pitting. A fundamental understanding of the materials science and electrochemistry of the nitrite role is expected to lead to superior and more cost-effective corrosion prevention methods for storing and processing complex, industrially important salt solutions. One important application of this new information in the DOE complex involves the high-level radioactive waste solutions contained in carbon steel tanks.

There is an extensive base of engineering knowledge of corrosion prevention by nitrite in alkaline salt solutions containing various organic and inorganic aggressive species. This knowledge is empirical; effective nitrite concentrations have been related to solution composition and temperature through numerous laboratory tests. The role of nitrite has not been explained electrochemically in a general manner that permits the prediction of nitrite effectiveness in solutions of widely varied composition.

The product of the proposed work is a model of the nitrite concentration required to prevent pitting corrosion in terms of the electrochemical and surface oxide properties of the carbon steel solution system for a wide range of solution compositions. Typical industrial salt solutions contain numerous ionic species and suspended insoluble compounds, as well as dissolved organic species.

Such complex solutions present a great challenge to modeling the electrochemical behavior of the alloys in which they are contained. We will develop the model in this program from experimental data obtained on the effects of significant corrosive anions (such as nitrate, sulfate and chloride) and the protective anion nitrite on the following:

- Various electrochemical potentials of steel in multicomponent industrial solutions
- The redox potential of the solutions
- The nature of the oxide film on steel exposed to the solutions.

We will apply modern, computer-controlled AC and DC electrochemical techniques to extract relevant electrochemical parameters. Using in-situ vibrational spectroscopy in specially designed cells, we will investigate the oxide film and its response to changes in the concentration of corrosive and protective species.

The program will be conducted at the DOE's Savannah River Site and at the University of South Carolina. The two organizations bring together extensive electrochemical testing experience and advanced electrochemical modeling experience.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

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"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm

Environmental Management Science Program Research in South Carolina

Clemson University

55052-SC - Advanced Sensing and Control Techniques to Facilitate Semi-Autonomous Decommissioning

Year of Award: 1996 **Amount of Award:** $870,733
Problem Area: Decontamination and Decommissioning
Science Category/SubCategory: Engineering Science / Robotics
Principal Investigator: Dr. Robert J. Schalkoff, 864-656-5913, rjschal@hubcap.clemson.edu
For More Information: http://www.doe.gov/em52/55052.html

Description Provided by Investigator:

This research is intended to advance the technology of semiautonomous teleoperated robotics as applied to Decontamination and Decommissioning (D&D) tasks. Specifically, research leading to a prototype dual-manipulator mobile work cell is proposed. This cell is supported and enhanced by computer vision, artificial intelligence and virtual reality technology. Key to this task is the synergistic use of vision algorithms to facilitate visual reasoning in uncertain and unstructured environments under telepresence (VR) control. Operator 'immersion' and the use of AI techniques facilitate disassembly. A three-year, three-phase effort is proposed, with demonstrations at the end of years 2 and 3. The availability of the work cell would enhance both worker productivity and protection in the D&D of hazardous sites. In addition, the underlying research is expected to advance the fusion of the technologies of quantitative computer vision, robotics, visualization and planning.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Decontamination and Decommissioning problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Decontamination and Decommissioning".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
§+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
§+ RL-ER06	C-141	Decontamination and Decommissioning
§+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
+ RL-TP07	C-161	Plutonium Finishing Plant (PFP) Vault Management

Environmental Management Science Program Research in South Carolina

Furman University

54828-SC - Processing of High Level Waste: Spectroscopic Characterization of Redox Reactions in Supercritical Water

Year of Award: 1996 **Amount of Award:** $109,000
Problem Area: Mixed Waste
Science Category/SubCategory: Inorganic Chemistry / Hydrothermal Oxidation
Principal Investigator: Dr. Charles A. Arrington, 864-294-3369, Arrington_Tony/furman@furman.edu
For More Information: http://www.doe.gov/em52/54828.html

Description Provided by Investigator:

Work is underway during the summer of 1997 at Los Alamos National Laboratory in collaboration with Steve Buelow of group CST-6 at LANL. Two undergraduate students are working with the principle investigator at LANL for 10 weeks.

Current efforts are focused on the oxidative dissolution of chromium compounds found in Hanford tank waste sludge. Samples of chromium oxides and hydroxides with varying degrees of hydration are being characterized using Raman, FTIR, and XPS spectroscopic techniques. Kinetics of oxidation reactions at subcritical and supercritical temperatures are being followed by Raman spectroscopy using a high temperature stainless steel cell with diamond windows. In these reactions both hydrogen peroxide and nitrate anions are used as the oxidizing species with Cr(III) compounds and organic compounds as reducing agents.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
+ RL-TW04	C-169	Retrieval Project
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
+ SR-HL02	C-253	F-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations

Environmental Management Science Program Research in South Carolina

University of South Carolina

55205-SC - A Fundamental Study of Laser-Induced Breakdown Spectroscopy Using Fiber Optics for Remote Measurements of Trace Metals

Year of Award: 1996 **Amount of Award:** $630,000
Problem Area: Remedial Action
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Laser Ablation Techniques
Principal Investigator: Dr. Scott Goode, 803-777-2601, goode@psc.psc.sc.edu
Major Collaborator(s): S. Michael Angel at the University of South Carolina
For More Information: http://www.doe.gov/em52/55205.html

Description Provided by Investigator:

Improved technologies are required by DOE for characterization and monitoring for site clean-up and waste processing applications. Especially needed are field deployable methods and devices of real-time monitoring to reduce dependency on laboratory analyses which are costly and time consuming. Improved sensors are needed for on-site analyses to provide real-time analytical capabilities for screening level and/or decision-quality data. Matrices of interest to the DOE are soils (or other solids), slurries, and aqueous and non-aqueous solutions.

Laser-induced breakdown spectroscopy (LIBS) is a useful method for determining the elemental composition of solids. This method has been recently reviewed and a number of different applications have been described. In the LIBS technique, a high-power pulsed laser is used to generate a plasma from the sample of interest. This phenomenon was first demonstrated in 1963 using a pulsed ruby laser. The elemental composition of the sample is accomplished by measuring the atomic emission from the atoms and ions in the plasma. There are many reports of the use of LIBS for measuring metals in solid substrates. There have also been LIBS investigations of aerosols, single particles, metals in solution including uranium, and even chlorinated species in solution. More recently, LIBS has been used for measuring Ba and Cr in soil using a fiber-optic cable. LIBS shows great potential for measuring metal contaminants in soils and on particles (e.g., stack emissions) based on their atomic emission in a laser-induced plasma. Another important application for this technique is the remote analysis of highly radioactive materials, such as the glasses produced by the Defense Waste Processing Facility. The use of fiber optics for both collection of the atomic emission and delivery of the laser to the sampling area could eliminate the need for sampling.

In this work we will study the time-evolution of the LIBS emission for different matrices to better understand how to optimize the signal. Also, we will investigate the use of fiber optics for laser delivery and signal collection, and the influence of the geometry of the fiber optic launch and collection probes to determine the effect on the signal-to-noise ratio (SNR). Finally, we will study the LIBS signal for different sample matrices as a function of excitation wavelength across a broad spectrum. A result of this study should be a determination of the optimal excitation and collection conditions and sampling times for metal contaminants in different matrices, and an understanding of the strengths and limitations of using fiber optics for LIBS sampling.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV212	C-49	Underground Test Area (UGTA)
§ NV214	C-53	Industrial Sites
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER02	C-129	200 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
ID-HLW-101	C-29	High-Level Waste Pretreatment
ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
+ RL-TW04	C-169	Retrieval Project
+ RL-TW05	C-173	Process Waste Support
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
+ RL-TW08	C-185	Process Waste Privatization Infrastructure
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
+ SR-HL01	C-249	H-Tank Farm
+ SR-HL02	C-253	F-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
SR-HL05	C-265	Vitrification
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in Tennessee

Oak Ridge National Laboratory

54973-TN - A Novel Energy-Efficient Plasma Chemical Process for the Destruction of Volatile Toxic Compounds

Year of Award: 1996 **Amount of Award:** $980,222
Problem Area: Mixed Waste
Science Category/SubCategory: Engineering Science / Bubble Mechanics and Sonification
Principal Investigator: Dr. Lal A. Pinnaduwage, 423-574-6540, llp@ornl.gov
For More Information: http://www.doe.gov/em52/54973.html

Description Provided by Investigator:

Removal of *low-concentrations (below several percent) of toxic volatile compounds from* contaminated air streams is encountered at DOE waste sites in two instances:(i) off-gases resulting from air-stripping of contaminated soils and (ii) effluent from the incineration of highly-concentrated combustible hazardous wastes. Due to the inefficiencies associated with thermal plasma treatment of such wastes, non-thermal plasma techniques are currently being pursued. Most of the non-thermal plasma processes involve the ionization/dissociation of the carrier-gas molecules (N_2 and O_2) via collisions with energetic electrons and subsequent interaction of radicals/ions thus produced with the target gas molecules; much of the electrical energy may be wasted in producing unused ions/radicals in the carrier gases. Therefore, we believe that these non-thermal processes are not very energy efficient, even though they offer an improvement over thermal plasma processes. We propose an innovative plasma chemical process that is based on extremely large electron attachment cross sections ($\geq 10^{-12}$ cm^2) recently discovered at ORNL for the *highly-excited electronic states of molecular species.* Furthermore, a discharge-based, *target-specific excitation process* (a novel plasma mixing scheme) is proposed for the excitation of target molecules.

The proposed novel approach, that exploits the new knowledge on electron attachment to highly-excited states and the old (but not yet exploited) knowledge on excitation transfer from rare-gas metastables, can be expected to yield significant time and cost reductions associated with *in situ* off-gas treatment of contaminated soils at DOE waste sites as well as in the secondary treatment of emissions from the incineration of combustible hazardous wastes. The ability of this process to "zero in" on target gases without wasting energy on the bulk of the carrier gases consisting of N_2 and O_2 should lead to significant cost savings.

An inherent requirement of the proposed studies is the ability to accurately determine the concentrations of the toxic components both at the reactor input (concentration levels anywhere from tens of ppm to a few percent), and at the output (concentrations down to below ppm). We will use proven analytical techniques to accurately assess the efficiency of the proposed destruction techniques. We plan to bring the proposed laboratory studies to a stage where they will be ready for pilot-scale demonstrations at the end of the three-year period.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW03	C-287	Mixed Low Level Waste Project
AL024	C-3	Grand Junction Office (GJO) All Other Projects
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ OR-48101	C-99	Offsite Remedial Action
+ OR-45301	C-103	Paducah Remedial Action
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
RL-ER08	C-147	Groundwater Management
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Tennessee

Oak Ridge National Laboratory

55013-TN - Biofiltration of Volatile Pollutants: Engineering Mechanisms for Improved Design, Long-term Operation, Prediction and Implementation

Year of Award: 1996 **Amount of Award:** $950,000
Problem Area: Remedial Action
Science Category/SubCategory: Engineering Science / Bioengineering
Principal Investigator: Dr. Brian H. Davison, 423-576-8522, davisonbh@ornl.gov
For More Information: http://www.doe.gov/em52/55013.html

Description Provided by Investigator:

This work seeks to produce industrial and EM-relevant scientific information for successful biofiltration operation in the following three ways:

1 . Fundamental methods will be developed to make long-term operation of biofilter units possible via innovative application of nutrient limitation and filter regeneration.

2. Biological and transport fundamentals will be incorporated into a nonsteady state mathematical model with extension to TCE, BTEX, and VOC removal in order to successfully predict operating parameters and thus enable advanced design a priori.

3. Enhancement of the biofiltration process will be achieved by incorporating cosolvents into the recirculating media and embedding high viscosity organics into the packing material.

Advances in these areas are particularly important for implementation and extended activity of biofilters in industrial settings and are directly relevant for high priority EM contaminants, including alkanes, aromatics, and chloroorganics. These tasks are part of the remediation by natural processes focus area, which addresses the broad class of volatile organic contaminants with applications to hydrocarbons. chlorinated hydrocarbons such as TCE, and nitrates. Specifically, this project researches the "emission-free destruction of organic wastes" through "off-gas treatment that eliminates emissions in the environment that exceeding [the] EPA. requirements [including] bioremediation." (EMSP Call. Notice 96-10. 1996). It directly addresses needs as listed in the EM-50 Rainbow Series.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§ RL-ER08	C-147	Groundwater Management
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Tennessee

Oak Ridge National Laboratory

55033-TN - Characterization of Chemically Modified Hyperthermophilic Enzymes for Chemical Syntheses and Bioremediation Reactions

Year of Award: 1996 **Amount of Award:** $1,393,000
Problem Area: Remedial Action
Science Category/SubCategory: Health Science / Molecular, Structural and Genomic Science
Principal Investigator: Dr. Eric N. Kaufman, 423-574-6624, ekn@ornl.gov
Major Collaborator(s): Michael Adams at the University of Georgia
For More Information: http://www.doe.gov/em52/55033.html

Description Provided by Investigator:

Research developments in the area of biocatalysis in organic solvents are expected to greatly expand the role of bioprocessing in chemical synthesis, fuel processing, and bioremediation technologies. Many biological transformation reactions of interest to DOE site remediation involve species that are only sparingly soluble in aqueous environments. Hence, destruction of these incalcitrant and toxic materials would benefit tremendously if their degradation could be performed in nonaqueous environments. Organic biocatalysis may be motivated by the nature of the substrate itself, or by augmented mass transport, ease of product recovery, or novel reaction pathways afforded by the organic solvent. For instance, polychlorinated biphenyls (PCB's), dense nonaqueous phase liquids (DNAPL's), and manufactured gas plant wastes are sparingly soluble in water, but may be more effectively processed when solubilized by organic liquids. However, naturally occurring enzymes are not soluble in organic solvents, indeed, most spontaneously denature and, depending on the solvent used, typically form inactive and insoluble precipitates.

The objective of the proposed work is to gain a fundamental understanding of the molecular and catalytic properties of enzymes that have been chemically modified so that they are soluble and catalytically active in pure organic solvents. Hydrogenases and redox proteins obtained from hyperthermophiles, which are organisms that grow near and above 100°C, will be investigated as model systems, and the lessons learned will be applied to other hyperthermophilic enzymes with bioremediation potential. The premise for this study is that thermostable enzymes which are both soluble and catalytically active in both water and in a range of organic solvents are optimally suited for bioremediation where substrates of interest are more soluble and may be processed with greater specificity in nonaqueous solvents.

This collaborative project brings together the very different yet complementary expertises from two institutions. The Oak Ridge National Laboratory has extensive experience in bioprocess engineering for fuels, chemicals and remediation, while the University of Georgia routinely grows several hyperthermophiles in large scale culture and from them has purified a variety of enzymes and proteins. This project utilizes the experience of both laboratories with the objective of producing a variety of solvent-soluble biocatalysts that are able to function at extreme temperatures for bioremediation reactions. We will investigate the physical and catalytic properties of chemically modified hyperthermophilic hydrogenases as model systems for biorefining reactions in organic solvents. We will also explore how the modified hydrogenase and other enzymes may be utilized in remediation reactions via novel reaction pathways that may be afforded through organic biocatalysis.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV214	C-53	Industrial Sites
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER02	C-129	200 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ RF014	C-213	Industrial Zone Closure Project
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II

Environmental Management Science Program Research in Tennessee

Oak Ridge National Laboratory

55036-TN - Colloid Transport and Retention in Fractured Deposits

Year of Award: 1996 **Amount of Award:** $1,100,000
Problem Area: Remedial Action
Science Category/SubCategory: Hydrogeology / Fluid-flow and Colloidal Dynamics
Principal Investigator: Dr. John F. McCarthy, 423-576-6606, jjj@ornl.gov
Major Collaborator(s): Paul Reimus at Los Alamos National Laboratory
Motomu Ibaraki at Ohio State University
Martha J. M. Wells at Tenessee Technological University
Larry McKay at the University of Tennessee
For More Information: http://www.doe.gov/em52/55036.html

Description Provided by Investigator:

A series of field-scale and laboratory-scale experiments, using both natural undisturbed samples and simple one-dimension "artificial fractures", are proposed to investigate the influence of physical and chemical factors on the transport of colloids in fractured materials (weathered shale saprolite and unweathered shale). The experimental results will be assessed using a computer model (COLFRAC) developed to simulate colloid transport in fractured materials. The overall goal is to assess the relative influence of chemical and physical factors expected to influence colloid transport in fractured materials and investigate strategies for predictive simulation at the field scale. The experimental methods each operate at different physical/geological scales and can be used with different degrees of experimental control. This allows testing of hypotheses in a relatively simple setting in the laboratory where individual chemical or colloidal characteristics can be varied, and then the results compared with field-scale experiments where the influence of realistic geologic heterogeneity can be incorporated. Understanding the processes that control colloid behavior will increase confidence with which colloid-facilitated contaminant transport can be predicted and assessed at various contaminated DOE sites. An added benefit is the expectation that this work will yield novel techniques to either immobilize colloid-bound contaminants in-situ, or mobilize colloids for enhancing remedial techniques such as pump-and-treat and bioremediation.

References

- *Transport of Colloids*

- McCarthy, J. F., and J. M. Zachara. 1989. Subsurface transport of contaminants: Binding to mobile and immobile phases in groundwater aquifers. Environ. Sci. Technol. 23:496-504 (feature article).
- McCarthy, J. F. and C. Degueldre. 1993. Sampling and characterization of groundwater colloids for studying their role in the subsurface transport of contaminants. IN J. Buffle and H. van Leeuwen (Eds.) Environmental Particles, Volume II. Lewis Publishers, Chelsea MI. Chapter 6, pp. 247-315.

- *Colloid-facilitated transport*

- Ibaraki, M. And E. A. Sudicky. 1995a. Colloid-facilitated transport in discretely fractured porous medium. I. Numerical formulation and sensitivity analysis. Water Resources Res. 31:2945-2960.
- Ibaraki, M. And E. A. Sudicky. 1995b. Colloid-facilitated transport in discretely fractured porous medium. II. Fracture network examples. Water Resources Res. 31:2961-2969.

- *Novel Techniques*

- McCarthy, J. F., and F. J. Wobber. 1993. Manipulation of Groundwater Colloids for Environmental Restoration. Lewis Publishers, Chelsea, MI. 320 p.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ AL007	C-7	Environmental Restoration
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV212	C-49	Underground Test Area (UGTA)
§ NV214	C-53	Industrial Sites
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
ID-HLW-101	C-29	High-Level Waste Pretreatment
+ RL-TW04	C-169	Retrieval Project
+ RL-TW05	C-173	Process Waste Support
+ SR-HL01	C-249	H-Tank Farm
+ SR-HL02	C-253	F-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Tennessee

Oak Ridge National Laboratory

55087-TN - Design and Synthesis of the Next Generation of Crown Ethers for Waste Separations: An Inter-Laboratory Comprehensive Proposal

Year of Award: 1996 **Amount of Award:** $1,920,000
Problem Area: High Level Waste
Science Category/SubCategory: Separations Chemistry / Ligand Design and Ion-exchange
Principal Investigator: Dr. Bruce A. Moyer, 423-574-6718, moyerba@ornl.gov
Major Collaborator(s): M.L. Dietz at Argonne National Laboratory
Benjamin P. Hay at Pacific Northwest National Laboratory
S. Alexandratos at the University of Tennessee
For More Information: http://www.doe.gov/em52/55087.html

Description Provided by Investigator:

A combined effort at Oak Ridge, Pacific Northwest, and Argonne National Laboratories and the University of Tennessee is proposed to design, synthesize, and characterize the next generation of crown ethers for metal-ion separations applicable to USDOE's environmental needs. This research combines three inter-dependent projects dealing with 1) molecular mechanics and ligand design, 2) solvent-extraction properties, and 3) resin-immobilized crowns. Despite impressive developments in the chemistry of crown ethers, factors such as the need for polar environments and "forcing" conditions, weak efficiency, and dependence on matrix anions limits their potential in separations. Exploiting advances in molecular mechanics, this research seeks accelerated progress through ligand design and synthesis coupled with testing of predictions via structural, spectroscopic, and separation techniques. New crown compounds will be studied in solvent-extraction and polymer systems, emphasizing ion-exchange features. Selectivity principles governing the binding of such ions as Li^+, Cs^+, Sr^{2+}, and Ra^{2+}, all of which have been identified as contaminants at USDOE sites, will be investigated. The partner laboratories have world-recognized programs in the area of crown ethers, solvent extraction, and ion exchange. Their cooperation under this research represents an unusual and extremely effective combination of unique resources.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§+ RL-TW04	C-169	Retrieval Project
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§+ SR-HL01	C-249	H-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
RF014	C-213	Industrial Zone Closure Project
+ SR-SW01	C-281	Consolidated Incinerator Facility
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in Tennessee

Oak Ridge National Laboratory

55103-TN - Utilization of Kinetic Isotope Effects for the Concentration of Tritium

Year of Award: 1996 **Amount of Award:** $1,354,000
Problem Area: Mixed Waste
Science Category/SubCategory: Separations Chemistry / Catalyst Chemistry and Waste Treatment
Principal Investigator: Dr. Gilbert M. Brown, 423-576-2756, gbn@ornl.gov
Major Collaborator(s): Thomas Meyer at the University of North Carolina
For More Information: http://www.doe.gov/em52/55103.html

Description Provided by Investigator:

The objective of this project is to develop methods for concentrating tritium in water based on large primary isotope effects in catalytic redox processes. A process will be developed to remove tritium from H_2O by concentrating it with respect to protio-water that can be employed on a variety of scales to address DOE's tritium contamination problems. Chemical cycles will be developed that produce high concentration factors for HTO and T_2O based on the discrimination of C-H and C-T bonds in oxidation reactions. H-T discrimination occurs as the tritium containing compound is oxidized in a step involving a transition metal oxidant. Strong primary kinetic isotope effects lead to the oxidation of C-H bonds in preference to C-T bonds, and this reaction leads to concentration of tritium in the organic compound. The reduced form of the transition metal compound can be electrochemically reoxidized so that the oxidation step can be made catalytic. An investigation of the kinetics and mechanism of the oxidation of a number of organic substrates by ruthenium (IV) oxo complexes has revealed large, primary kinetic isotope effects. The proposed ruthenium oxo catalysts will be prepared, and their reactivity will be tested in a small bench-scale electrochemical reactor to demonstrate the individual steps required for the concentration of tritium in water. C-H/C-T kinetic isotope effects in the oxidation of organic substrates will then be evaluated, and the catalytic tritium enrichment of organic substrates will be demonstrated. Much of the work in the initial phase will involve evaluating various catalyst/substrate combinations including a determination of the desirability of binding an insoluble catalyst to the electrode surface. A second phase of the project will entail evaluating the chemistry for incorporation of deuterium and tritium into organic substrates preferably using an electrochemical reduction process that will involve HTO (or T_2O) as the source of tritium. The final phase of the project will involve development of a closed cycle bench scale system to concentrate tritium from groundwater.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW03	C-287	Mixed Low Level Waste Project
+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
RL-ER08	C-147	Groundwater Management
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Tennessee

Oak Ridge National Laboratory

55108-TN - Monitoring Genetic & Metabolic Potential for In Situ Bioremediation: Mass Spectrometry

Year of Award: 1996 **Amount of Award:** $1,080,000
Problem Area: Remedial Action
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Biomedical Instrumentation
Principal Investigator: Dr. Michelle V. Buchanan, 423-574-4868, buchananmv@ornl.gov
For More Information: http://www.doe.gov/em52/55108.html

Description Provided by Investigator:

A number of DOE sites are contaminated with mixtures of dense non-aqueous phase liquids (DNAPLs) such as carbon tetrachloride, chloroform, perchloroethylene, and trichloroethylene. At many of these sites, in situ microbial bioremediation is an attractive strategy for cleanup, since it has the potential to degrade DNAPLs in situ without producing toxic byproducts. A rapid screening method to determine broad range metabolic and genetic potential for contaminant degradation would greatly reduce the cost and time involved in assessment for in situ bioremediation, as well as for monitoring ongoing bioremediation treatment. In this project, advanced mass-spectrometry-based methods will be developed at ORNL by Drs. Michelle Buchanan, Greg Hurst, and Scott McLuckey in the Organic Mass Spectrometry Group to screen for genetic and metabolic potential and for metabolic activity for both assessment and monitoring of in situ bioremediation of DNAPLs. The proposed work builds on proof-of-principle experiments already completed in our group that demonstrated detection of relevant microbial PCR products by matrix-assisted laser desorption/ionization (MALDI) mass spectrometry and detection of polar metabolites associated with bioremediation by electrospray mass spectrometry. In work described in a companion proposal (Monitoring Genetic and Metabolic Potential for In Situ Bioremediation: Microbiology), Professor Mary Lidstrom of the University of Washington will identify small DNA sequences specific for processes of importance to biodegradation and apply the new MS-based methods to detection of metabolites associated with DNAPL bioremediation. By working in close collaboration, these two groups will optimize and extend these methods to increase their sensitivity and broaden their applicability. This work will lay the foundation for development of a field-portable mass-spectrometry based technique for rapid assessment and monitoring of bioremediation processes on site.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§ RL-ER08	C-147	Groundwater Management
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Tennessee

Oak Ridge National Laboratory

55119-TN - Phase Equilibria Modification by Electric Fields

Year of Award: 1996 **Amount of Award:** $1,202,000
Problem Area: Remedial Action
Science Category/SubCategory: Inorganic Chemistry / Multiphase/Gaseous Chemistry
Principal Investigator: Dr. Costas Tsouris, 423-241-3246, tq9@ornl.gov
Major Collaborator(s): Vinod Shah at the University of Tennessee
For More Information: http://www.doe.gov/em52/55119.html

Description Provided by Investigator:

The primary focus of this program is to obtain a fundamental understanding of the effects of electric fields on polar and nonpolar mixtures in gas and liquid phases, with the ultimate goal of using this understanding in devising novel means to dramatically improve existing environmental remediation technologies and to develop new technologies. Based on preliminary experiments that showed a significant effect of electric fields on vapor-liquid equilibria, this program will investigate the thermodynamic equilibria, as well as transport properties, of multiphase systems under the influence of electric fields. Uniform and nonuniform electric fields will be applied across an interface to modify the composition of the bulk fluids adjacent to the interface. Studies will be focused on understanding the phenomena involved and quantifying the effects in vapor-liquid and liquid-liquid equilibria. Dielectric spectroscopy will be used to study nonlinear dielectric effects of electric fields, infrared and Raman spectroscopy will be used to study hydrogen bonding and molecular association, and surface light scattering will be used to study interface properties. Concentration measurements in the bulk phases will determine the magnitude of equilibria modification. It is expected that this program will lead to greater efficiency in a wide range of environmental treatment processes, including extraction, sorption, and stripping. These processes are widely used by DOE for treatment of wastes and sites contaminated with heavy metals, radionuclides, and organic chemicals, particularly in the SUB-CON and Mixed Waste Focus Areas.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ AL024	C-3	Grand Junction Office (GJO) All Other Projects
§ NV214	C-53	Industrial Sites
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ OR-48101	C-99	Offsite Remedial Action
§+ OR-45301	C-103	Paducah Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ RF014	C-213	Industrial Zone Closure Project
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
ID-HLW-101	C-29	High-Level Waste Pretreatment
ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
+ RL-TW04	C-169	Retrieval Project
+ RL-TW05	C-173	Process Waste Support
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW08	C-185	Process Waste Privatization Infrastructure
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
+ SR-HL01	C-249	H-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
SR-HL05	C-265	Vitrification
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in Tennessee

Oak Ridge National Laboratory

55267-TN - Containment of Toxic Metals and Radionuclides in Porous and Fractured Media: Optimizing Biogeochemical Reduction versus Geochemical Oxidation

Year of Award: 1996 **Amount of Award:** $1,235,006
Problem Area: Remedial Action
Science Category/SubCategory: Biogeochemistry / Biogeochemistry
Principal Investigator: Dr. Philip M. Jardine, 423-574-8058, ipj@ornl.gov
Major Collaborator(s): James Saiers at Florida International University
John Zachara at Pacific Northwest National Laboratory
Scott Fendorf at the University of Idaho
For More Information: http://www.doe.gov/em52/55267.html

Description Provided by Investigator:

The overall goal of this research is to provide an improved understanding and predictive capability of the mechanisms that allow metal-reducing bacteria to be effective in the bioremediation of subsurface environments contaminated with toxic metals and radionuclides. The study is motivated by the likelihood that subsurface microbial activity can effectively alter the redox state of toxic metals and radionuclides so that they are immobilized for long time periods. Our objectives are to (1) develop an improved understanding of the rates and mechanisms of competing geochemical oxidation and microbiological reduction reactions that govern the fate and transport of redox-sensitive metals and radionuclides in the subsurface, and (2) quantify the conditions that optimize the microbial reduction of toxic metals and radionuclides, for the purpose of contaminant containment and remediation in heterogeneous systems that have competing geochemical oxidation, sorption, and organic ligands. The proposed work consists of three multidisciplinary tasks that build upon existing collaborations established within DOE's Subsurface Science Program. Our approach involves the use of (a) a dynamic flow technique to quantify the geochemical oxidation and microbial reduction rates and mechanisms controlling the mobility of uranium (U), chromium (Cr), and cobalt-EDTA (Co-EDTA) in pure mineral oxides and in heterogeneous soils/sediments, (b) novel spectroscopic techniques to monitor the time-dependent redox transformation and immobilization of U, Cr, and Co-EDTA by subsurface media, and (c) a high performance supercomputer model that couples hydrologic-biogeochemical transport processes for simulation of the experimental data. The experimental and numerical results of this research will quantify the conditions that optimize the microbial reduction of contaminant metals for the purpose of contaminant stabilization in heterogeneous systems. Our research findings will contribute directly to on-going or planned remediation efforts at Hanford's *In Situ* Redox Manipulation site, Savannah River's Old Burial Ground site, and Oak Ridge's Y-12 sites. By providing an improved understanding and predictive capability of competitive geochemical processes that affect biological metal reduction, we will enhance the successful application of microbially mediated contaminant stabilization in the field. Further, this research combines DOE's commitment to environmental restoration with its commitment to major facilities (synchrotron sources and high performance supercomputing) and academic education.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ AL007	C-7	Environmental Restoration
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV214	C-53	Industrial Sites
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Tennessee

Oak Ridge National Laboratory

55276-TN - Fundamental Chemistry and Thermodynamics of Hydrothermal Oxidation Processes

Year of Award: 1996 **Amount of Award:** $1,220,000
Problem Area: Mixed Waste
Science Category/SubCategory: Inorganic Chemistry / Hydrothermal Oxidation
Principal Investigator: Dr. John M. Simonson, 423-574-4962, xxs@ornl.gov
For More Information: http://www.doe.gov/em52/55276.html

Description Provided by Investigator:

The purpose of this research is to determine experimentally the fundamental thermodynamic and phase-equilibrium properties which control inorganic chemical reactions in high-temperature aqueous solutions as directly related to the assessment of technology and avoidance of problems in treatment of DOE hazardous and mixed wastes by hydrothermal oxidation (HTO). Models suitable for interpolation and limited extrapolation of these results will be developed to extract the maximum possible fundamental insights from the experimental values, and to insure the broadest possible applicability of the experimental studies to a wide variety of HTO operating conditions. A significant part of this modeling activity will involve molecular-scale simulation of solution properties through molecular dynamics simulations over wide ranges of state conditions.

New experimental information will be obtained on the solubility of solids (including radionuclides), the compositions of multiple coexisting fluid phases, and the physical properties of these fluids over the wide ranges of state variables characteristic of HTO systems. These new data will be combined with appropriate existing experimental results and treated quantitatively using a new modeling framework developed in this research. In addition, microscopic (molecular-scale) properties of aqueous solutions at high temperatures will be elucidated through molecular dynamics simulations; these simulation results will be used to guide the extrapolation of phenomenological models.

Benefits to DOE include an improved understanding of the fundamental chemistry and thermodynamics of aqueous solutions at high temperatures, and the experimental information and data-analysis tools needed to assess the potential application of HTO technology for the destruction of DOE aqueous mixed waste.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW03	C-287	Mixed Low Level Waste Project
NV214	C-53	Industrial Sites
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Tennessee

Oak Ridge National Laboratory

59978-TN - Thermospray Mass Spectrometry Ionization Processes Fundamental Mechanisms for Speciation, Separation and Characterization of Organic Complexants in DOE Wastes

Year of Award: 1997 **Amount of Award:** $590,000
Problem Area: High Level Waste
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Mass Spectrometry
Principal Investigator: Dr. John E. Caton, 423-241-5189, jec@ornl.gov
For More Information: http://www.doe.gov/em52/59978.html

Description Provided by Investigator:

In order to understand the equilibria of organic complexants and their products in multi-component mixtures this task will develop and interpret positive and negative ion thermospray mass spectra of complexants and complexant products using liquid chromatography combined with thermospray mass spectrometry. The approach will be in two phases:

1. Thermospray mass spectrometry for complexors and their products with metals (including radionuclides) will be investigated at ORNL in order to define the chemical species in aqueous media. A parallel task at the University of Minnesota will investigate liquid chromotography on inert stationary phases to facilitate the introduction of individual chemical species or simplified mixtures into the mass spectrometer.

2. The knowledge from Phase 1 will be used to demonstrate the principles and approaches required to effect the determination of equilibria and the evaluation of the impact of complexants on waste treatment.

New knowledge will be generated by successes in these proposed studies and DOE will realize practical benefits:

a. in waste disposal where the concentration of organic complexers is required by waste acceptance criteria;

b. in waste treatment where DOE EM-50 sponsors efforts to destroy chelators and to remove metal species from wastes; and

c. in decontamination and decommissioning where chelating agents (used in cleaning) must be removed from the waste stream.

Specific DOE needs for waste characterization tools (Hanford Site Science Need: (RL-WT038-S) and for determining the effect of organic constituents on waste processing (RL-WT058-S) will also benefit.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§+ RL-TW04	C-169	Retrieval Project
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
ID-WM-107	C-45	Long Term Treatment/Storage/Disposal Operations
RL-WM03	C-193	Solid Waste Storage and Disposal
RL-WM04	C-197	Solid Waste Treatment
+ SR-SW02	C-285	Transuranic Waste Project
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in Tennessee

Oak Ridge National Laboratory

60020-TN - Stability of High-Level Waste Forms

Year of Award: 1997 **Amount of Award:** $762,000
Problem Area: High Level Waste
Science Category/SubCategory: Materials Science / Chemical and Structural Properties Of Storage Materials
Principal Investigator: Dr. Theodore M. Besmann, 423-574-6852, tmb@ornl.gov
For More Information: http://www.doe.gov/em52/60020.html

Description Provided by Investigator:

The assessment of release of radionuclides from waste repositories substantially depends on the leaching behavior of the spent fuel or waste form. Assumed rates based on dissolution of specific phases (assumption of unit activity) will lead to potentially grossly overestimated values as well as possibly underestimated values, and are therefore difficult to defend. Current, experimentally determined values are less than desirable since they depend on measurement of the leach rate under non-realistic conditions designed to accelerate processes that are geologic in time scale. With the possible consideration of a hot repository for the disposal of spent fuel and high-level waste forms, the materials will experience elevated temperatures (> 100 C) for hundreds of years or longer, driving chemical and phase changes. The objective of the effort is to develop a basic understanding of the phase equilibria and solid solution behavior of the constituents of high-level waste forms and to model that behavior. The results of this effort will provide reaction path information for leaching/transport codes such as ESP, as well as basic insights into complex ceramic solution behavior, bonding in glasses, and crystal chemistry of the fluorite-structure uranium dioxide-fission product system.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§ ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§+ RL-TW08	C-185	Process Waste Privatization Infrastructure
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§ SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Tennessee

Oak Ridge National Laboratory

60037-TN - Estimation of Potential Population Level Effects of Contaminants on Wildlife

Year of Award: 1997 **Amount of Award:** $618,901
Problem Area: Health / Ecology / Risk
Science Category/SubCategory: Health Science / Risk Assessment
Principal Investigator: Dr. Bradley E. Sample, 423-241-3933, pz7@ornl.gov
For More Information: http://www.doe.gov/em52/60037.html

Description Provided by Investigator:

Although risk managers for CERCLA sites are concerned with risks to wildlife *populations*, methods for wildlife risk assessments are based on effects on *individuals*. The purpose of this project is to provide DOE with methods to assess risks to wildlife populations. We propose a series of tasks, culminating in the integration of contamination exposure-response function with species-specific population models for estimating the population-level effects associated with individual-level contaminant exposure. First, we will develop a database of dose-response functions for contaminants of concern to DOE EM. These toxicity data represent the foundation of all future work, because, to accurately interpret the significance of incremental increases in contaminant exposure, toxicity must be expressed as a function of exposure and not simple threshold values, as is the current practice. Because toxicity data are not available for all contaminants or wildlife species that may be considered in an ecological risk assessment, our second task will be to investigate and develop improved approaches for inter-species extrapolation of toxicity data. Our third task is to develop and parameterize matrix-based population models for selected wildlife species. When integrated with the contaminant exposure-response distributions, the population models will provide a tool to estimate population-level effects associated with differing levels of exposure and to compare these effects to other sources of mortality and environmental stresses. The issues of density dependence, spatial heterogeneity, stochasticity, and community-level interactions will be addressed for a subset of these species. The tasks outlined in this research are intended to reduce uncertainty associated with wildlife risk assessments. These uncertainties may have direct impacts on DOE EM satisfactorily fulfilling its mission in two ways. First, toxicity values may be too conservative. Risks to wildlife may therefore be overstated and remediation recommended when it is not needed. Second, some toxicity values may not be adequately protective and risks to wildlife may therefore be understated and remedial actions are not recommended when they are needed. Either of these alternatives results in inefficient use of limited EM funds and leaves DOE vulnerable to potential NRDA liability.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Health / Ecology / Risk problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Health / Ecology / Risk".

Environmental Management Science Program Research in Tennessee

Oak Ridge National Laboratory

60077-TN - Development of Nuclear Analysis Capabilities for DOE Waste Management Activities

Year of Award: 1997 **Amount of Award:** $600,000
Problem Area: Nuclear Materials
Science Category/SubCategory: Engineering Science / Design, Process and Modeling
Principal Investigator: Dr. Cecil V. Parks, 423-574-5280, cvp@ornl.gov
For More Information: http://www.doe.gov/em52/60077.html

Description Provided by Investigator:

This research involves research and development in support of complementary technologies that are required to fulfill the anticipated needs of the DOE in its charter to safely provide for the management and ultimate disposition of nuclear facilities and materials. Specifically, the research incudes the utilization of novel computational techniques, improved nuclear data, and new analytical methods to address criticality safety issues of interest to the Office of Environmental Management in its ongoing activities to dispose of DOE-owned spent nuclear fuel, and to assure criticality safety of fissile materials during facility remediation. In particular, the work will concentrate on the research and development necessary for: (1) utilization of sensitivity and uncertainty methods for the determination of computed margins of subcriticality and safety for fissile material in waste matrices; and (2) formulation of arbitrary-grid radiation transport methods to facilitate calculations on a broad range of problem domains and for the complex geometric configurations typical of DOE research and weapons processing facilities. Enhancement of computational capabilities in these areas would simultaneously address three criteria important to the DOE mission: improved safety resulting from a more thorough understanding of underlying physical phenomena, optimization of fissile material operations resulting in reduced costs, and expedited performance as a consequence of improved efficiency and defensibility in safety analyses and reviews.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Nuclear Materials problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Nuclear Materials".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ RL-TP07	C-161	Plutonium Finishing Plant (PFP) Vault Management

Environmental Management Science Program Research in Tennessee

Oak Ridge National Laboratory

60197-TN - Microsensors for In-situ Chemical, Physical, and Radiological Characterization of Mixed Waste

Year of Award: 1997 **Amount of Award:** $615,000
Problem Area: Remedial Action
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Sensors and Techniques
Principal Investigator: Dr. Thomas G. Thundat, 423-574-6201, ugt@ornl.gov
For More Information: http://www.doe.gov/em52/60197.html

Description Provided by Investigator:

A widespread need exists for portable, real-time, in-situ chemical, physical, and radiological sensors in characterization of mixed waste, groundwater, contaminated soils and process streams. None of the currently available technologies offer a clear path to the development of sensors that are miniature, cost-effective, selective, highly sensitive with a wide dynamic range, and with the ability to work in air or liquid while providing chemical, physical, and radiological information. We propose an innovative single-sensor platform approach that is based on the recently discovered extreme sensitivity of microcantilever sensing using adsorption-induced forces.

The objective of this research program is to gain a better understanding of the basic mechanism of adsorption-induced differential surface stress variation and to use this novel idea for developing sophisticated microsensor concepts for sensing in liquids. As a demonstration we will develop: (i) chemically specific microsensors by coupling surface modification chemistry with molecular recognition agents for identification of inorganic species found in groundwater, (ii) coating techniques that will enable operation in corrossive, and high ionic strength environment, and (iii) microcantilevers for assessing local radioisoptope content based on radiation damage.

This new multipurpose sensor technology offers the potential to provide real-time, in-situ characterization of the chemical, physical, and radiological properties of groundwater, contaminated soils and process streams. The advantage of this approach is that once the basic technique is developed, it can be the basis for a universal sensor platform for many DOE needs such as the chemical, physical, and radiological characterization of tank waste, monitoring of environmental cleanup processes, and the detection of emitted gases from incinerators and waste vitrification plants.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ AL024	C-3	Grand Junction Office (GJO) All Other Projects
§ AL007	C-7	Environmental Restoration
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV212	C-49	Underground Test Area (UGTA)
§ NV214	C-53	Industrial Sites
§ OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
§+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ OR-45301	C-103	Paducah Remedial Action
§+ OR-46301	C-107	Portsmouth Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER02	C-129	200 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ RF014	C-213	Industrial Zone Closure Project
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
ID-WM-107	C-45	Long Term Treatment/Storage/Disposal Operations
+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
+ RL-TP07	C-161	Plutonium Finishing Plant (PFP) Vault Management
+ RL-TW04	C-169	Retrieval Project
+ RL-TW05	C-173	Process Waste Support
+ RL-TW07	C-181	Process Waste Privatization Phase II
RL-WM03	C-193	Solid Waste Storage and Disposal
RL-WM04	C-197	Solid Waste Treatment
+ SR-HL01	C-249	H-Tank Farm
+ SR-HL02	C-253	F-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
SR-HL05	C-265	Vitrification
SR-NM06	C-273	Nuclear Materials Storage
+ SR-SW01	C-281	Consolidated Incinerator Facility
+ SR-SW02	C-285	Transuranic Waste Project
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in Tennessee

Oak Ridge National Laboratory

60217-TN - Optically-Based Array Sensors for Selective In Situ Analysis of Tank Waste

Year of Award: 1997 **Amount of Award:** $600,000
Problem Area: High Level Waste
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Sensors and Techniques
Principal Investigator: Dr. Gilbert M. Brown, 423-576-2756, gbn@ornl.gov
For More Information: http://www.doe.gov/em52/60217.html

Description Provided by Investigator:

Fundamental research will be directed toward developing an array of chemically selective sensors, based on highly selective molecular recognition agents and fluorescence techniques, coupled to fiber optics, for the safe and cost-effective in situ characterization of high level waste tanks. Characterization of high level tank waste currently entails obtaining and analyzing core samples at the cost of about $1 million per sample. The ability to detect and measure specific chemicals and radionuclides directly inside a high level waste tank using a remote sensing device could result in considerable benefits with regard to both cost savings and safety issues. This multidisciplinary approach to the design of sensors will be to immobilize agents for selective molecular recognition, chosen from solvent extraction processes, in an organic polymer matrix that mimics the organic medium in an aqueous-nonaqueous extraction. In this manner the matrix will enhance both the separation and the achievement of chemical selectivity. Complexation of Cs by derivatives of calix-crown ether ligands containing a fluorophore designed to exhibit an increase in the emission intensity upon metal ion complexation will serve as a means of detecting this element. By also using ligands that are selective for Na or K in separate sensor elements, a correction for the interference can be obtained. We will use an array of sensor sites, each with optimized selectivity for one of the components in the analyte, attached to an imaging fiber optic bundle. Ligand design, synthesis, and evaluation will be conducted during the first year of the project, with the development of sensor sites on fiber optics being conducted largely during the second and third years. Any deficiencies in selectivity, arising from cross reactivity for competing ions, will be overcome by using pattern recognition algorithms to deconvolute the array's response.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§+ RL-TW04	C-169	Retrieval Project
§+ RL-TW05	C-173	Process Waste Support
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
§ SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Tennessee

Oak Ridge National Laboratory

60218-TN - Novel Mass Spectrometry Mutation Screening for Contaminant Impact Analysis

Year of Award: 1997 **Amount of Award:** $600,000
Problem Area: Health / Ecology / Risk
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Biomedical Instrumentation
Principal Investigator: Dr. Chung Hsuan (Winston) Chen, 423-574-5895, che@ornl.gov
For More Information: http://www.doe.gov/em52/60218.html

Description Provided by Investigator:

This research addresses the DNA mutation due to the exposure to contaminated media and to promote a better understanding of the relationship between exposure and health impact which are among the top priorities in the Environmental Management Science Program (EMSP). The capability of rapid mutation screening is essential for sound risk analysis for various contamination sites. However, rapid DNA mutation screening technology is still not available. Our objective is to develop innovative mass spectrometry technology to achieve fast mutation screening from contaminated area and to reveal the linkage between gene mutation and contaminants. Mass spectrometry has the potential to achieve very fast speed sample analysis. However, the poor mass resolution and low detection efficiency for long DNAs limit the broad application for mutation screening. In this program, new innovative approaches for improving mass resolution and detection sensitivity will be pursued to achieve rapid DNA screening. Allele specific polymerase chain reaction (ASPCR) will be coupled with the proposed novel mass spectrometry for detecting DNA mutations. At completion of the technology development, the merit of our approach will be directly tested by analyzing the possible mutations in ras gene wildlife, such as fish, exposed to environmental genotoxic agents. Successful accomplishment of the program will allow that genotoxic effect of hazardous waste to be routinely assessed directly at DNA level at an affordable cost.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Health / Ecology / Risk problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Health / Ecology / Risk".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
NV214	C-53	Industrial Sites
+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
OR-43204	C-77	ORNL Bethel Valley Deactivation and Decommissioning
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RF014	C-213	Industrial Zone Closure Project
+ SR-SW01	C-281	Consolidated Incinerator Facility

University of Tennessee

55083-TN - Behavior of Dense, Immiscible Solvents in Fractured Clay-Rich Soils

Year of Award: 1996 **Amount of Award:** $599,947
Problem Area: Remedial Action
Science Category/SubCategory: Hydrogeology / Dense Non-Aqueous Phase Liquid (DNAPL) Dynamics
Principal Investigator: Dr. Larry D. McKay, 423-974-2366, LMCKAY@UTK.EDU
Major Collaborator(s): Philip Jardine at Oak Ridge National Laboratory
John A. Cherry at the University of Waterloo
For More Information: http://www.doe.gov/em52/55083.html

Description Provided by Investigator:

A series of laboratory-scale experiments on the behavior of dense, immiscible solvents (commonly referred to as DNAPL's) in large diameter, undisturbed columns of fractured clay till and highly weathered and fractured shale saprolite are proposed. The lab studies will focus on the influence of fracture aperture/spacing/distribution and/or matrix porosity on factors such as DNAPL entry pressures, distribution of DNAPL residual, dissolution of residual and diffusion into the high porosity matrix. These results will be compared to field-scale investigations of existing DNAPL contamination at several sites in these same materials. The undisturbed column samples will be taken at two research sites, one in southwestern Ontario and the other near Oak Ridge, TN, that have been exceptionally well characterized and have been the location of numerous investigations on groundwater flow and solute or colloid transport. The sites for field investigations of existing DNAPL contamination are located close to the previous research sites and are in the same deposits, allowing for comparison of results at both field- and lab-scales. Information from the laboratory and field studies will be compared to results of mathematical simulations using models that have been recently developed to specifically examine the problem of DNAPL's in fractured, high porosity deposits.

The two types of deposits are widespread in the eastern U.S. and underlie Federal sites such as the Fernald site in Ohio and the Oak Ridge Reservation in Tennessee. Although of different origin, they share many common characteristics (fracture-controlled flow, high matrix porosity) and have remarkably similar behavior with respect to contaminant transport. Previous theoretical investigations and a few preliminary laboratory experiments indicate that DNAPL behavior in these types of deposits will be dramatically different than in granular deposits, influencing both assessment/monitoring and potential for remediation of DNAPL contamination. The research will systematically examine key factors involved in DNAPL behavior in fractured, high porosity deposits and has the potential to substantially improve our understanding and capability of dealing with such contamination.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ NV212	C-49	Underground Test Area (UGTA)
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Tennessee

University of Tennessee

55328-TN - Novel Analytical Techniques Based on an Enhanced Electron Attachment Process

Year of Award: 1996 **Amount of Award:** $540,000
Problem Area: Remedial Action
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Sensors and Techniques
Principal Investigator: Dr. Lal A. Pinnaduwage, 423-574-6540, llp@ornl.gov
Major Collaborator(s): Dr. Michelle V. Buchanan at Oak Ridge National Laboratory
For More Information: http://www.doe.gov/em52/55328.html

Description Provided by Investigator:

Present analytical methodologies for the detection of chlorinated compounds important to DOE's environmental restoration program, such as DNAPLs [dense non-aqueous phase liquids--such as carbon tetrachloride, trichloroethylene (TCE), perchloroethylene (PCE)], polychlorinated biphenyls (PCB), and others, involve detection by negative-ion-based analytical techniques. These techniques exploit electron attachment to *analyte molecules in their ground electronic states,* and are limited to particular compounds with appropriate electron capture cross sections (> about 10^{-17} cm^2). For example, PCB contamination is detected by analysis of mixtures of chlorinated homologues of these biphenyls. Homologues with lower numbers of chlorines do not efficiently attach thermal electrons and thus are not detected by either electron capture chromatographic detectors or by negative ion chemical ionization mass spectrometry.

A basic research program recently conducted by the PI has shown that *highly-excited electronic states of molecules* have electron attachment cross sections of ≥ *10^{-12} cm^2, orders of magnitude larger compared to electron attachment cross sections for ground-state molecules.* Furthermore, this enhanced electron attachment process appears to occur in a *wide variety of molecules,* in contrast, electron attachment to ground-state molecules -- which the present negative-ion-based analytical techniques rely on-- is limited to certain classes of molecules. We propose three novel analytical techniques based on this enhanced negative-ion formation process.

In one of the proposed techniques, the excited states of the (analyte) molecules are populated via laser excitation; the resulting negative ions are mass analyzed for identification. Preliminary results using this technique show that analytically useful fragment negative ions can be produced with this technique in molecules which do not produce any negative ions in conventional analytical methods.

However, more studies are needed to assess the usefulness of the new technique. (Using this apparatus positive-ion spectra can be recorded as well, thus providing complementary information).

The other two proposed techniques utilize a specialized gas discharge for the formation of excited species (and low-energy electrons for attachment), and thus will provide a cost-effective method if successful; in one version the negative ions will be mass analyzed -- as in the laser-based technique -- and in the other the decrease in electron density due to excited state attachment will be monitored (electron capture detector mode). A plasma mixing scheme will be employed to excite the analyte molecules (they will not be directly subjected to the discharge) so that the excited states of the analyte molecules will not be destroyed by the discharge.

We plan to bring the proposed laboratory studies to a stage where they will be ready for field study demonstrations at the end of the three-year period.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

Environmental Management Science Program Research in Tennessee

University of Tennessee

60096-TN - Rational Synthesis of Imprinted Organofunctional Sol-Gel Materials for Toxic Metal Separation

Year of Award: 1997 **Amount of Award:** $450,000
Problem Area: Mixed Waste
Science Category/SubCategory: Separations Chemistry / Ligand Design and Ion-exchange
Principal Investigator: Dr. Ziling (Ben) Xue, 423-974-3443, xue@novell.chem.utk.edu
Major Collaborator(s): Dr. Sheng Dai at Oak Ridge National Laboratory
For More Information: http://www.doe.gov/em52/60096.html

Description Provided by Investigator:

Current cost estimates for the environmental remediation of contaminated installations under the auspices of the Department of Energy (DOE) are staggering. On this basis alone, there is a critical need to develop the scientific basis for new approaches to the treatment and disposal of toxic metal ions from wastes or contaminated areas at many DOE sites.

The overall goal of this project is to rationally design and synthesize imprinted, hybrid inorganic-organic sol-gel materials containing metal binding sites through template approaches, and to develop a scientific basis for metal ion binding and recognition by such tailored hybrid inorganic-organic materials. After removal of the template M, functionalized cavities are created which contain both grafted binding sites and functionality inherent to the silica network (Si-OH, Si-O-Si). These cavities are expected to "recognize" and bind the target metal ions through the high affinities between the binding sites and M, and their retained shapes. Our approaches utilize both the metal ion binding and the tailored impressions of the template metal ions in the imprinted cavities. Such imprinted organofunctional sol-gel networks are expected to exhibit both high selectivity and capacity for binding targeted ions in fluid waste streams.

The principles of sol-gel chemistry and imprinting techniques will guide our approaches to optimize the chemical and physical properties of the imprinted organofunctional sol-gel materials. Cold isotopes or non-radioactive surrogate ions of similar size and charge will be used in imprinting investigations to minimize hazardous waste production. The design strategy we will follow is based on imprinted binding sites cross-linked by rigid, hydrophilic inorganic SiO_2 or $M'O_2$ networks. These hydrophilic metal oxide-based materials are expected to exhibit fast ion mass transfer and binding kinetics in comparison to functionalized hydrophobic organic polymers.

Success in this research will lead to a novel class of materials tailored for toxic metal recognition/separation with enhanced capacity and selectivity. It will also provide the scientific basis for such recognition and the development of a new generation of technologies for more efficient toxic metal removal. Furthermore, these research results should be directly applicable to DOE Environmental Management (EM) missions.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW03	C-287	Mixed Low Level Waste Project
ID-HLW-101	C-29	High-Level Waste Pretreatment
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-TW04	C-169	Retrieval Project
+ RL-TW05	C-173	Process Waste Support
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RF014	C-213	Industrial Zone Closure Project
+ SR-HL01	C-249	H-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Texas

Rice University

60115-TX - Advanced High Resolution Seismic Imaging, Material Properties Estimation and Full Wavefield Inversion for the Shallow Subsurface

Year of Award: 1997 **Amount of Award:** $550,100
Problem Area: Remedial Action
Science Category/SubCategory: Geophysics / Subsurface Imaging
Principal Investigator: Dr. Alan Levander, 713-527-6064, alan@geophysics.rice.edu
For More Information: http://www.doe.gov/em52/60115.html

Description Provided by Investigator:

We propose to develop and test an integrated suite of imaging and inverse techniques appropriate to the range of wave propagation regimes customarily recorded in shallow seismic surveys. These techniques will address the extreme physical conditions found in the shallow environment, and thereby significantly advance the ability of shallow seismic investigations to produce high fidelity structural and material property maps of the subsurface. High resolution subsurface material properties maps are essential for characterizing the geometry of aquifers, aquicludes, and other fluid pathways, and therefore are essential for environmental remediation efforts.

We will apply these methods to a number of high resolution profiles we have acquired and are proposing to acquire at sites with different near surface properties, including two active environmental remediation sites. The methods to be developed represent basic research in seismic imaging, and include advanced wavefield imaging using pre-critical to post-critical energy, velocity estimation and reflector focusing, and wavefield inversion techniques appropriate for imaging and estimating the material properties of the highly heterogeneous near surface environment. The research will build on the PIs' previous research developing seismic imaging and inversion methods tailored for petroleum exploration and crustal investigations. At all stages of the data processing we propose to exploit the entire wavefields commonly recorded (and often overlapping in time, space, frequency, and phase velocity) but customarily processed and interpreted independently in high resolution surveys.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

Environmental Management Science Program Research in Texas

Texas A&M University

54735-TX - Development of Inorganic Ion Exchangers for Nuclear Waste Remediation

Year of Award: 1996 **Amount of Award:** $599,999
Problem Area: High Level Waste
Science Category/SubCategory: Separations Chemistry / Ligand Design and Ion-exchange
Principal Investigator: Dr. Abraham Clearfield, 409-845-2936, pjf2434@acxrd.chem.tamu.edu
Major Collaborator(s): J. L. Collins at Oak Ridge National Laboratory
Dr. B. Zane Egan at Oak Ridge National Laboratory
For More Information: http://www.doe.gov/em52/54735.html

Description Provided by Investigator:

This research is concerned with the development of highly selective inorganic ion exchangers for the removal of primarily Cs^+ and Sr^{2+} from nuclear tank waste and from groundwater. In this study, we will probe the, origins of selectivity through detailed structural studies and the thermodynamics of the ion exchange processes. The compounds to be synthesized may have cavity or tunnel structures, layer structures, or be amorphous gels. In our previous work, we have prepared highly selective Cs^+ and Sr^{2+} sorbents, including a new family of alkali metal group 4(14) polysilicates. The structures of one of the polysilicates and titanium silicates with tunnel structures have been solved by *ab initio* powder methods and refined by Rietveld techniques. We have then probed the ion exchange process by preparing the protonated form of the exchanger and refined the structure at different levels of ion uptake. At the same time, NMR spectra of ^{29}Si were obtained. These studies revealed the intimate details of the ion exchange process and similar procedures will be applied to the crystalline exchangers exhibiting high selectivities. It has been observed that the selectivities, particularly of the exchangers with tunnel structures, can be significantly altered by framework substitution and by the degree of crystallinity built into the exchangers. Therefore, systematic substitutions of framework ions based on ionic radii and charge will be carried out, and their effect on selectivity determined. Crystallinity will be controlled by the time, temperature, and pressure of synthesis. These studies will be used to predict the thermodynamics of exchange and tested by carrying out measurements of their thermodynamic properties ($\Delta G°$, $\Delta H°$,$\Delta S°$, K).

The starting point of our research is conditioned by our previous studies in which highly selective exchangers for Cs^+ and Sr^{2+} have already been prepared, including the polysilicates, pharmacosiderites, and other silicates with tunnel structures, micas, and brittle micas for immobilization of ions in soils, layered titanates as strontium sorbers, and pillared clays and titanates. In addition, over a 30 year period we have synthesized many families of exchangers that can be applied to specific problems involving Pb^{2+} , Cd^{2+}, Hg^{2+}, Co^{2+}, etc. contamination. In order to be aware of these problems and to be able to apply our studies to real waste problems, we propose a collaboration with Oak Ridge National Laboratory personnel who are engaged in actual waste cleanup problems. They are experts in producing inorganic exchangers in usable engineered forms and in column studies.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§+ RL-TW04	C-169	Retrieval Project
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
§ SR-HL05	C-265	Vitrification
AL024	C-3	Grand Junction Office (GJO) All Other Projects
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ OR-48101	C-99	Offsite Remedial Action
+ OR-45301	C-103	Paducah Remedial Action
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
RL-ER08	C-147	Groundwater Management
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project
+ SR-SW01	C-281	Consolidated Incinerator Facility
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in Texas

Texas A&M University

55115-TX - The Adsorption and Reaction of Halogenated Volatile Organic Compounds (VOC's) on Metal Oxides

Year of Award: 1996 **Amount of Award:** $390,000
Problem Area: Mixed Waste
Science Category/SubCategory: Inorganic Chemistry / Solid/Solution Chemistry
Principal Investigator: Dr. Jack Lunsford, 509-845-3455, lunsford@chemvx.chem.tamu.edu
For More Information: http://www.doe.gov/em52/55115.html

Description Provided by Investigator:

The goal of the research is to elucidate the properties of the material responsible for the activation of halocarbons and the nature of the intermediates formed in the dissociative adsorption of this general class of compounds. This information is essential for interpreting and predicting stoichiometric and catalytic pathways for the safe destruction of halocarbon pollutants. The specific research objectives are: (1) to study the adsorption and reactivity of chloromethanes, chloroethanes, and chloroethylenes on basic, neutral, and acidic oxides, including magnesium oxide, chromium oxide, silica, alumina, silica-alumina, and iron and cobalt oxides, both supported and unsupported; (2) to identify the reaction intermediates of the above halocarbons by Raman spectroscopy, NMR methods, and infrared reflection absorption and high resolution electron energy loss spectroscopies (IRAS and HREELS, respectively); (3) to define rate laws and kinetic models for the reaction of the above halocarbons with O_2 on oxides surfaces; (4) to investigate the effect of H_2O on the selectivity with respect to formation of Cl_2 and HCl; and (5) to determine the role of adsorbed oxygen and chlorine as poisons for halocarbon activation on oxides.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
+ OR-46301	C-107	Portsmouth Remedial Action
RL-ER08	C-147	Groundwater Management
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Texas

University of Texas at Austin

54506-TX - Acid-Base Behavior in Hydrothermal Processing of Wastes

Year of Award: 1996 **Amount of Award:** $379,620
Problem Area: Mixed Waste
Science Category/SubCategory: Inorganic Chemistry / Hydrothermal Oxidation
Principal Investigator: Dr. Keith P. Johnston, 512-471-4617, kpj@che.utexas.edu
For More Information: http://www.doe.gov/em52/54506.html

Description Provided by Investigator:

The cost of High Level Waste (HLW) disposal can be lowered, substantially by reducing the volume requiring vitrification and long term storage. For the Hanford Tank Wastes, chromium and radioactive compounds can be oxidized to produce soluble forms that can be separated from other sludge components. In a preliminary study, Los Alamos National Laboratories has demonstrated the feasibility of treating these wastes with a new technology, hydrothermal oxidation (also called supercritical water oxidation). The nitrates are reduced to nitrogen; furthermore, phosphates, alumina sludge, and chromium are solubilized and the sludge is reconstituted as fine oxide particles. Organic carbon is converted to CO_2 and metals to the highest oxidation state, which enhances their solubility for separation.

A major obstacle to development of this technology has been a lack of scientific knowledge of the solution chemistry and thermodynamics. Extremely little is known presently due to severe experimental challenges. Nevertheless. because water at high temperatures is highly compressible, the density can vary over a large range with conditions, and the dielectric constant can range from 1.5 to 10; correspondingly, large variations in ion solvation and acid-base equilibria are expected. Consequently, changes in these properties will have a profound effect on the key issues in hydrothermal technology: waste destruction efficiency, salt solubility, metal-ion complexation, acid-base catalysis of hydrolysis and oxidation reactions, and reactor corrosion.

To develop this new branch of acid-base chemistry in water above 325°C and to achieve breakthroughs which could make hydrothermal oxidation a successful technology for the Department of Energy, our objectives are to develop a fundamental molecular understanding of the thermodynamics of ion solvation and acid-base equilibria and how they affect metal-ion complexation and salt solubility and to use this information to develop easily implemented but molecular-based models. Furthermore, we will study ionic transport behavior and corresponding simplified models for the correlation of transport coefficients with conditions and ionic character.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

Environmental Management Science Program Research in Texas

University of Texas at Austin

55185-TX - New Strategies for Designing Inexpensive but Selective Bioadsorbants for Environmental Pollutants: Selection of Specific Ligands & Their Cell Surface Expression

Year of Award: 1996 **Amount of Award:** $749,392
Problem Area: Remedial Action
Science Category/SubCategory: Health Science / Molecular, Structural and Genomic Science
Principal Investigator: Dr. Brent L. Iverson, 512-471-5053, biverson@utxvms.cc.utexas.edu
Major Collaborator(s): Mohammad Ataai at the University of Pittsburg
For More Information: http://www.doe.gov/em52/55185.html

Description Provided by Investigator:

Bacteria will be produced that have peptides or antibodies on the surface capable of binding toxic metal species with very high affinity. These bacteria will be used to maker bioadsorbents, which will be characterized in detail.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ AL024	C-3	Grand Junction Office (GJO) All Other Projects
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV214	C-53	Industrial Sites
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ OR-46301	C-107	Portsmouth Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ RF014	C-213	Industrial Zone Closure Project
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
OR-43204	C-77	ORNL Bethel Valley Deactivation and Decommissioning
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation

Environmental Management Science Program Research in Texas

University of Texas at Austin

55216-TX - In-Situ Characterization of Dense Non-Aqueous Phase Liquids Using Partitioning Tracers

Year of Award: 1996 **Amount of Award:** $600,000
Problem Area: Remedial Action
Science Category/SubCategory: Hydrogeology / Dense Non-Aqueous Phase Liquid (DNAPL) Dynamics
Principal Investigator: Dr. Gary A. Pope, 512-471-3235, Gary_Pope@pe.utexas.edu
Major Collaborator(s): Akhil Datta-Gupta at Texas A&M University
For More Information: http://www.doe.gov/em52/55216.html

Description Provided by Investigator:

Problem Definition and Importance

Non-aqueous phase liquids (NAPLs) exist in many unsaturated (vadose) and saturated zones and act as long term sources of groundwater contamination. NAPLs are found in a wide variety of hydrogeological environments beneath federal facilities throughout the U.S. Of paramount concern are NAPLs which are denser than water (DNAPLs), in particular chlorinated hydrocarbons such as trichloroethene (TCE), tetrachloroethene (PCE), carbon tetrachloride (CTET) and polychlorinated biphenyls (PCBs), which have been identified beneath many DOE facilities. Also of concern are light NAPLs (LNAPLs) such as fuel hydrocarbons, which have proven easier to characterize than DNAPLs because of their buoyancy. Quantifying the amount and spatial distribution of NAPL trapped in porous media at hazardous waste sites is of great importance in determining its environmental impact and in selecting appropriate remediation alternatives. This research will focus on the issue of DNAPL characterization, although the methodology is just as applicable to LNAPLs as to DNAPLs.

Problem Difficulties

In the last 15 years of hydrogeological practice, several methods have been developed for characterizing dissolved-phase plumes of contaminants. However, no reliable, quantitative method (with the exception of the technology described herein) has been developed to characterize the zone containing DNAPL. Conventional coring methods provide point measurements of contaminant concentrations and require interpolation of often sparsely distributed data to estimate total NAPL volumes in the flow domain. The number of sampling locations is usually limited by cost, including the high cost of obtaining the cores and subsequent laboratory analysis for contaminant concentrations. There are several other limitations to coring methods that are site specific and will not be discussed here, but are nevertheless serious problems under some circumstances. Studies of residual DNAPL distribution in heterogeneous, sandy aquifer materials indicate that cores are unlikely to provide reliable estimates of the volume of DNAPL at the field scale because the representative elementary volume of residual DNAPL appears to be much larger than that provided by cores (Mayer and Miller, 1992) It has now become desirable to move away from reliance on core samples alone to estimate DNAPL volumes in the subsurface and to use interwell tests to estimate the residual or pooled DNAPL volumes over meaningful distances (Jin *et al.,* 1995; Wilson and MacKay, 1995).

Proposed Solution

During the past three years, a new technology for characterizing DNAPL zones has been developed by The University of Texas at Austin and INTERA, Inc. of Austin and successfully applied at two federal hazardous waste sites by the authors of this proposal (Pope *et al.,* 1994; Annable *et al.,* 1995; Butler *et al.,* 1995; Jin *et al.,* 1995; Pope *et al,* 1995; Whitley *et al.,* 1995; Jin *et al.,* 1996; Studer *et al.,* 1996). The technology is known as a partitioning interwell tracer test (PITT) and employs asuite of conservative and reactive or "partitioning" tracers which are introduced into a well or wells located in the subsurface beneath a hazardous waste site and subsequently extracted from other wells. During the transport of the tracers by advecting air or ground water through the interwell zone, the partitioning tracers are retarded in their transport by interaction with any DNAPL present while the conservative tracers are not retarded. The chromatographic separation of the tracers indicates the presence of DNAPL in the interwell zone and is used to determine the volume of DNAPL present. Laboratory scale batch and column tests have shown the potential use of both long-chain alcohols and fluorocarbons (Jin *et al.,* 1995; Jin *et al.,* 1996; Dwarakanath *et al.*, 1996) as partitioning tracers for quantifying NAPL content in the saturated zone of aquifers, and the use of perfluorocarbons for accomplishing the same in the vadose zone (Whitley *et al.*, 1995).

PITT technology has been used since the early 1970's to measure the volume of residual oil present in petroleum reservoirs (Zemel, 1995). However, most of these tests were single-well tests rather than the interwell tests that are the focus of this proposal. Furthermore, there are many significant differences in conditions between the oil field and the aquifer tests proposed here and many fundamental scientific questions remain to be addressed before this technology can be used in the widest possible range of contaminated aquifer conditions. PITTs have several advantages over conventional soil sampling and analysis. The use of partitioning tracers provides a spatially integrated measure of the NAPL volume present in the tracer flow domain. Since the test is based on the flow-field in contact with the NAPL, the tracer test results can be used for the design of physical, chemical or biological remediation methods that target the NAPL source region using adjuvants delivered by fluids. Thus, the PITT has the potential of saving enormous amounts of time and money by focusing the expensive remediation fluids on the NAPL source.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Vermont

University of Vermont

54931-VT - A Novel Biomarker for Beryllium Sensitization in Humans

Year of Award: 1996 **Amount of Award:** $432,608
Problem Area: Health / Ecology / Risk
Science Category/SubCategory: Health Science / Molecular, Structural and Genomic Science
Principal Investigator: Dr. Richard J. Albertini, 802-656-8866, ralberti@zoo.uvm.edu
Major Collaborator(s): Donna Cragle at Oak Ridge Associated Universities
L. Gayle Littlefield at Oak Ridge Associated Universities
For More Information: http://www.doe.gov/em52/54931.html

Description Provided by Investigator:

This research project will determine the T-cell receptor (TCR) gene usages of beryllium reactive T-lymphocytes isolated directly from the peripheral blood of individuals exposed at a U.S. Department of Energy site. The objective is to develop a sensitive and novel biomarker for identifying early human sensitization to environmental beryllium. This is a collaborative project involving the Genetics Laboratory of the University of Vermont and both the Center for Epidemiological Research and the scientific staff of the Cytogenetics Program at the Oak Ridge Institute for Science and Education (ORISE). The > 2000 beryllium exposed workers who have been contacted for participation in the ORISE study "Follow-up of Beryllium Workers at the Y-12 Plant/Efficacy of the Peripheral Blood Lymphocyte Proliferation (LPT) and other Non-Invasive Procedures for Diagnosis of Chronic Beryllium Disease" will provide the pool of potential participants for the proposed study. Beryllium reactive T-lymphocytes will be directly isolated from peripheral blood using a novel antigen-independent method of surrogate selection for *in vivo* arising *hprt* mutants as representatives of clones that are undergoing chronic proliferation. The T-cells undergoing chronic proliferation in beryllium sensitized individuals will be enriched for beryllium reactive cells. The TCR β gene usage of these T-cell isolates will be determined and their junctional (CDR3) regions sequenced. Beryllium reactive T-cell clones will also be recovered following *in vitro* beryllium stimulation of peripheral blood lymphocytes from these same individuals and the TCR gene CDR3 region sequences similarly determined. The TCR β genes used by the beryllium reactive isolates and their CRD3 region sequences will be compared within*(in vivo* vs. *in vitro* derived) and among individuals with attention to kinds and durations of beryllium exposure and HPA DPB Glu 69 status. A method for quantitating total body loads of these antigen reactive T-cells in individuals will be developed using quantitative polymerase chain reaction (Q-PCR) amplification of specific TCR gene sequences. Successful achievement of this overall objective will permit future studies aimed at the elucidation of the immunological mechanisms underlying sensitization, the comparison of cells involved in pulmonary and systemic sensitization and the definition of potential targets for immunotherapy.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Health / Ecology / Risk problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Health / Ecology / Risk".

Environmental Management Science Program Research in Vermont

University of Vermont

60069-VT - Least-Cost Groundwater Remediation Design Using Uncertain Hydrogeological Information

Year of Award: 1997 **Amount of Award:** $372,845
Problem Area: Remedial Action
Science Category/SubCategory: Hydrogeology / Instrumentation and Modelling
Principal Investigator: Dr. George F. Pinder, 802-656-8697, pinder@uvm-gen.emba.uvm.edu
For More Information: http://www.doe.gov/em52/60069.html

Description Provided by Investigator:

The project seeks to examine the importance of uncertainty in hydraulic conductivity in the least-cost design of groundwater contamination containment systems. The problem is defined through the specification of inward gradient constraints or target concentration constraints along the three-dimensional envelope that defines the contaminant plume. At selected locations along this envelope Either the minimum acceptable inward gradient required to adequately assure flow into the plume or target concentration constraints are specified. From a preselected set of well locations, a subset of these locations is identified and pumping rates assigned by the optimization algorithm. The selection process is such as to achieve the minimum pumpage consistent with satisfying the constraints.

The unique aspects of this formulation are the use of a new conceptual approach to the accommodation of aquifer parameter uncertainty in optimal groundwater remediation design and the introduction of a new operations-research technique to solve this optimization problem.

The new approach, called robust optimization, has not heretofore been used to solve the above defined problem. It allows for the determination of a Robust, lowest-possible cost, pumping design that is consistent with the inherent uncertainty in the hydraulic conductivity field. It also allows for the visualization of how one can trade off excess pumping for enhanced security (decreased risk).

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ OR-46301	C-107	Portsmouth Remedial Action
§ RL-ER08	C-147	Groundwater Management
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Washington

Pacific Northwest National Laboratory

54621-WA - Chemical Speciation of Strontium, Americium, and Curium in High Level Waste: Predictive Modeling of Phase Partitioning During Tank Processing

Year of Award: 1996 **Amount of Award:** $1,050,778
Problem Area: High Level Waste
Science Category/SubCategory: Actinide Chemistry / Actinide (Heavy Element) Chemistry
Principal Investigator: Dr. Andrew R. Felmy, 509-372-6296, ar_felmy@ccmail.pnl.gov
Major Collaborator(s): Gregory Choppin at Florida State University
For More Information: http://www.doe.gov/em52/54621.html

Description Provided by Investigator:

Current strategies for reducing the total volume of radioactive tank waste requiring disposal at Hanford and other DOE sites call for the development of methods to selectively dissolve and remove non-radioactive elements such as Al, P, and Cr while retaining or precipitating the radioactive elements, including Sr and the actinide elements, in the tank sludges. This partitioning between solids and precipitates is fundamentally dependent upon the chemical speciation of the elements present in the tank processing solutions. Pacific Northwest National Laboratory and Florida State University propose a multidisciplinary research program designed to address the problem of trivalent actinide and strontium speciation and solubility in HLW tank supernatants. This approach will focus on the changes in speciation of Sr and Am/Cm in the presence of four key organic chelates and how changes in hydrolysis and carbonate complexation under high base conditions compete with these organic chelates and alter the speciation of the metal ions. This approach will take advantage of new advances in analytical instrumentation as well as computational chemistry methods (density functional theory) to begin to address fundamental problems in aqueous speciation such as how to determine the concentrations of individual metal-chelate or metal-chelate-hydroxide species present in solutions containing several different competing metal ions and chelators. This information on chemical speciation will then be used, in conjunction with certain necessary thermodynamic measurements, to develop thermodynamic models that will allow the prediction of changes in chemical speciation and solubility which can occur in response to changes in tank processing conditions. In this way we can both develop new approaches that address fundamental problems in aqueous speciation and at the same time provide useful and practical information needed for tank processing.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§+ RL-TW04	C-169	Retrieval Project
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
§ SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Washington

Pacific Northwest National Laboratory

54628-WA - Colloidal Agglomerates in Tank Sludge: Impact on Waste Processing

Year of Award: 1996 **Amount of Award:** $1,788,000
Problem Area: High Level Waste
Science Category/SubCategory: Inorganic Chemistry / Solid/Solution Chemistry
Principal Investigator: Dr. Bruce C. Bunker, 509-375-5969, bc_bunker@ccmail.pnl.gov
Major Collaborator(s): William A. Hamilton at Oak Ridge National Laboratory
Dr. James E. Martin at Sandia National Laboratories - Albuquerque
John C Berg at the University of Washington
For More Information: http://www.doe.gov/em52/54628.html

Description Provided by Investigator:

During processing of radioactive wastes, insoluble sludges consisting of submicron colloidal particles can clog transfer lines or interfere with solid-liquid separations. The wide range of properties observed for tank wastes can be rationalized by understanding how solution conditions influence the agglomeration of these colloidal particles. In the research, experiments will be performed on well defined colloidal suspensions of tank waste components to: 1) understand the nature and strength of interparticle forces leading to agglomeration, 2) define the relationships between interparticle forces and agglomerate structures, 3) establish the impact that agglomerate structures have on the rheology and sedimentation properties of colloidal suspensions, and 4) explore methods for manipulating agglomerate structures to optimize tank waste processing conditions. The work connects basic science at the particle level to macroscopic properties of interest to process design engineers, providing a technically defensible strategy for handling existing tank waste-related problems and for evaluating a wide range of processing options under consideration by both the DOE and industry.

INTRODUCTION

Disposal of millions of gallons of existing radioactive wastes is a major remediation problem for the Department of Energy. Although radionuclides are the most hazardous waste constituents, the components of greatest concern from a waste processing standpoint are insoluble sludges consisting of submicron colloidal particles. Depending on processing conditions, the colloidal particles can form agglomerate networks that can clog transfer lines or interfere with solid-liquid separations such as settle-decant operations. Under different conditions, the particles can be dispersed to form fines that will not sediment in settle-decant steps and that can foul and contaminate downstream components including ion exchangers or filtration systems.

Given the wide range of tank chemistries present at Hanford and other DOE sites, it is impractical to measure the properties of all tank wastes under all potential processing conditions in order to design rational treatment procedures. Instead, a framework needs to be established to allow property trends to be predicted on a sound scientific basis. The scientific principles of greatest utility in characterizing, understanding, and controlling the physical properties of sludge suspensions fall in the realm of colloid chemistry.

Objectives of this research are to:

1. Understand the factors controlling the nature and extent of colloidal agglomeration under expected waste processing conditions.

2. Determine how agglomeration phenomena influence physical properties relevant to wasteprocessing including, rheology, sedimentation, and filtration.

3. Develop strategies for optimizing processing conditions via control of agglomeration phenomena.

Below is a brief description of:

- proposed tank waste processing steps that are impacted by the presence of colloidal sludges
- physical properties of concern in tank waste processing
- scientific issues in agglomeration that can be used to rationalize the physical properties of colloidal suspensions
- specific research activities that are proposed for understanding and exploiting colloidal phenomena to deal with DOE's waste remediation problems.

The results of this work will enhance existing understanding of agglomeration phenomena and the properties of complex colloidal suspensions. In addition, the work will aid in the development of new methods and techniques for processing the millions of gallons of hazardous tank wastes at various DOE sites.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

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Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§+ RL-TW04	C-169	Retrieval Project
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
§ SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Washington

Pacific Northwest National Laboratory

54635-WA - Molecular-Level Process Governing the Interaction of Contaminants with Iron and Manganese Oxides

Year of Award: 1996 **Amount of Award:** $1,450,000
Problem Area: Remedial Action
Science Category/SubCategory: Geochemistry / Sorption/Desorption
Principal Investigator: Dr. Scott A. Chambers, 509-375-2220, sa_chambers@ccmail.pnl.gov
Major Collaborator(s): Dr. Gordon E. Brown at Stanford University
For More Information: http://www.doe.gov/em52/54635.html

Description Provided by Investigator:

Many of the inorganic and organic contaminants present in sediments at DOE sites can be altered or destroyed by reduction and oxidation (redox) reactions occurring at mineral surfaces. A fundamental understanding of such redox processes provided by molecular-level studies on structurally and compositionally well-defined mineral surfaces will lead to: (i) improved models of contaminant fate and transport in geochemical systems, and, (ii) optimized manipulation of these processes for remediation purposes. To contribute to this understanding, we will study, both experimentally and theoretically, redox processes involving three important contaminants - chromate ion ($CrO_4{}^{-2}$), carbon tetrachloride (CCl_4), and trichloroethene (TCE, $ClHC{=}CCl_2$) - on the following iron and manganese oxides - hematite (α-Fe_2O_3), magnetite (Fe_3O_4), maghemite ((γ-Fe_2O_3), and pyrolusite (β-MnO_2).

These oxides and their hydroxylated analogs commonly occur as coatings on minerals or as interfaces in the subsurface environment. Single-crystal surfaces of these oxides will be synthesized in carefully controlled fashion by molecular beam epitaxy. These surfaces, as well as high surface area powdered samples of these oxides, will be used in spectroscopic and kinetic experiments in both aqueous and gas phases. Our goal is to identify products and to determine the kinetics and mechanisms of surface-catalyzed redox reactions of Cr(VI) and Cr(III), and the reductive dechlorination of CCl4 and TCE. The combination of theory and experiment will provide the base information needed to scale from the molecular level to the microscopic grain level minerals.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

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"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ AL007	C-7	Environmental Restoration
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV212	C-49	Underground Test Area (UGTA)
§ NV214	C-53	Industrial Sites
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ RF014	C-213	Industrial Zone Closure Project
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
OR-43204	C-77	ORNL Bethel Valley Deactivation and Decommissioning

Environmental Management Science Program Research in Washington

Pacific Northwest National Laboratory

54646-WA - Interfacial Radiolysis Effects in Tank Waste Speciation

Year of Award: 1996 **Amount of Award:** $871,389
Problem Area: High Level Waste
Science Category/SubCategory: Inorganic Chemistry / Solid/Solution Chemistry
Principal Investigator: Dr. Thomas M. Orlando, 509-375-6404, tm_orlando@pnl.gov
For More Information: http://www.doe.gov/em52/54646.html

Description Provided by Investigator:

The purpose of this program is to deliver pertinent, though sometimes basic, information which can be used to make rational decisions on safety issues and processing strategies associated with mixed waste clean-up. In particular, we will establish an understanding of radiolysis in mixed-phase systems typical of DOE heterogenous, radioactive/chemical wastes. This is an important scientific concern with respect to understanding tank waste chemistry issues which has received relatively little attention. We will demonstrate the importance of understanding solid-state radiolysis, secondary electron interactions, charge-transfer dynamics and the general effect of heterogenous solids (interface and particulate surface chemistry) on tank waste radiation processes. In particular, we will specifically address *i.) the role of solid-state and interfacial radiolysis in the generation of noxious gases, ii.) the mechanisms of organic compound degradation (i.e., the TBP problem at Savannah River), iii.) scientific issues underlying safe interim storage and iv.) the general effects of colloid surface-chemical properties on waste chemistry.* We also intend to provide basic information on non-thermal interfacial processes which should help facilitate the development of novel non-thermal processing technologies. An additional important result of our work will be the development of an integrated team of scientists who will be available to the DOE to help review tank safety concerns and safety response actions by DOE contractors.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

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"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ RL-TW04	C-169	Retrieval Project
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations

Environmental Management Science Program Research in Washington

Pacific Northwest National Laboratory

54672-WA - Radiation Effects in Nuclear Waste Materials

Year of Award: 1996 **Amount of Award:** $2,880,000
Problem Area: High Level Waste
Science Category/SubCategory: Materials Science / Radiation Effects On Storage Materials
Principal Investigator: Dr. William J. Weber, 509-375-2299, wj_weber@ccmail.pnl.gov
Major Collaborator(s): R. B. Bircher at Argonne National Laboratory
Michael A. Nastasi at Los Alamos National Laboratory
Dr. Rodney C. Ewing at the University of Michigan
For More Information: http://www.doe.gov/em52/54672.html

Description Provided by Investigator:

The objective of this multidisciplinary, multi-institutional research effort is to develop a fundamental understanding at the atomic, microscopic, and macroscopic levels of radiation effects in glass and ceramics that provides the underpinning science and models for evaluation and performance assessments of glass and ceramic waste forms for the immobilization and disposal of high-level tank waste, plutonium residues and scrap, surplus weapons plutonium, and other actinides. Studies will focus on the effects of ionization and elastic-collision interactions on defect production, defect interactions, structural rearrangements, diffusion, solid-state phase transformations, and gas accumulation using actinide containing materials, gamma irradiation, ion-beam irradiation and electron-beam irradiation to simulate the effects of alpha decay and beta decay on nuclear waste glasses and ceramics. This program will exploit a variety of structural, optical, and spectroscopic probes to characterize the nature and behavior of the defects, defect aggregates, and phase transformations. Computer simulation techniques will be used to determine defect production from ballistic and ionization interactions, calculate defect stability, energies of formation and migration, damage processes within an alpha-recoil cascade, and defect/gas diffusion and interaction. A number of irradiation facilities and capabilities will be used, including user facilities at several national laboratories, to study *in situ* the effects of irradiation under different conditions.

Introduction

Stabilization and immobilization of high-level waste (HLW) in storage tanks, high-level sludge in fuel storage basins, and plutonium residues/scraps are some of the largest and most costly challenges facing the U.S. Department of Energy (DOE) in its effort to close the nuclear fuel cycle and cleanup the DOE weapons complex. In addition, the immobilization and disposal of surplus weapons-grade plutonium creates growing technological demands that are historically and technically tied to DOE's environmental management and restoration activities. The immobilization and disposal of HLW and Pu is also a global issue, as other countries address the issues of surplus weapons Pu and continue to produce HLW from the reprocessing of commercial nuclear fuels. In most cases, these nuclear wastes will be immobilized in glass or alternatively, ceramic waste forms prior to permanent disposal. **A key challenge in the permanent disposal of HLW and Pu is the development of predictive models, which are based on a sound scientific understanding of relevant phenomena, thus allowing the assessment of long-term performance.** Radiation effects from β-decay of the fission products and α-decay of the actinides can potentially impact the long-term performance of glass or ceramic waste forms. **For all these waste forms, there is a critical lack of fundamental understanding on the effects of radiation on glasses and ceramics from the atomic to the macroscopic levels that prevents meaningful predictions of performance.** Because of this lack of basic understanding on radiation-damage processes, the limited existing data bases cannot be extrapolated to larger doses, lower dose rates, different temperature regimes, or different compositions. **For glasses proposed for the immobilization and disposal of the DOE high-level tank waste, the primary issues are related to the direct and synergistic effects of ionizing radiation from β-decay on the glasses. In the case of glasses and ceramics for the immobilization and disposal of Pu and other actinides (or high-actinide wastes), the primary issues are related to the effects of high-radiation dose and helium accumulation from α-decay.**

The Pacific Northwest National Laboratory (PNNL) will lead a coordinated, multiproject research effort based on a multidisciplinary, multi-institutional approach to develop a fundamental understanding of radiation effects in glasses and ceramics relevant to the immobilization and disposal of HLW, Pu residues/scraps, surplus weapons-grade Pu, and other actinides.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§ ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
§+ RL-TW04	C-169	Retrieval Project
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§+ RL-TW08	C-185	Process Waste Privatization Infrastructure
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
§ SR-HL05	C-265	Vitrification
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
+ RL-TP07	C-161	Plutonium Finishing Plant (PFP) Vault Management
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in Washington

Pacific Northwest National Laboratory

54679-WA - Architectural Design Criteria for F-Block Metal Ion Sequestering Agents

Year of Award: 1996 **Amount of Award:** $1,800,000
Problem Area: Mixed Waste
Science Category/SubCategory: Actinide Chemistry / Actinide (Heavy Element) Chemistry
Principal Investigator: Dr. Benjamin P. Hay, 509-372-6239, bp_hay@ccmail.pnl.gov
Major Collaborator(s): Dr. David M. Roundhill at Texas Tech University
Robert Treat Paine Jr at the University of New Mexico
For More Information: http://www.doe.gov/em52/54679.html

Description Provided by Investigator:

The objective of this project is to provide the means to optimize ligand architecture for f-block metal recognition. Our strategy builds on an innovative and successful molecular modeling approach in developing polyether ligand design criteria for the alkali and alkaline earth cations. The hypothesis underlying this research is that differences in metal ion binding with multidentate ligands bearing the same number and type of donor groups are primarily attributable to intramolecular steric factors. We will quantify these steric factors through the application of molecular mechanics models.

The research involves close integration of theoretical and experimental chemistry. The experimental work entails synthesizing novel ligands and experimentally determining structures and binding constants for metal ion complexation by series of ligands in which architecture is systematically varied. The theoretical work entails using electronic structure calculations to parameterize a molecular mechanics force field for a range of metal ions and ligand types. The resulting molecular mechanics force field will be used to predict low energy structures for unidentate, bidentate, and multidentate ligands and their metal complexes through conformational searches. Results will be analyzed to assess the relative importance of several steric factors including optimal M-L length, optimal geometry at the metal center, optimal geometry at the donor atoms (complementarity), and conformation prior to binding (preorganization). An accurate set of criteria for the design of ligand architecture will be obtained from these results. These criteria will enable researchers to target ligand structures for synthesis and thereby dramatically reduce the time and cost associated with metal-specific ligand development.

Background and Significance

Critical tasks in the cleanup of U.S. Department of Energy (DOE) sites include processing radioactive wastes for disposal in long-term storage, remediation/restoration of environmental sites resulting from radioactive contamination, and decontamination/decommissioning of nuclear facilities. Because the radioactive components, most of which are metals, are typically present in very low concentrations, it is desirable to remove them from the bulk of the contaminated source (process waste stream, groundwater, soil) and concentrate them to minimize the volume of radioactive material destined for permanent subsurface disposal and thus minimize disposal costs. One group of radionuclides, the actinides, which are pervasive throughout the DOE complex, is of special concern. In particular, thorium, uranium, neptunium, plutonium, americium, and curium with half-lives ranging from 10^2 to 10^6 years can all be found in various DOE wastes, contaminated soils and groundwaters, and contaminated facilities. Lanthanide elements are also of concern because they form an important group of fission products that can persist in radioactive wastes for decades (e.g., ^{152,154,155}Eu).

As the cleanup problem continues to be defined and regulatory limits continue to decrease, ever-increasing demands will be placed on separation technologies for metallic radionuclides. Several successful processes have been developed to separate actinides and lanthanides from specific matrices. It is important to note, however, that the variable oxidation states of the actinide metals and the diversity of waste streams ensure there is no universal separation process for all f-block radionuclides. Processes must be tailored to fit the waste constituents and form.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW03	C-287	Mixed Low Level Waste Project
ID-HLW-101	C-29	High-Level Waste Pretreatment
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW05	C-173	Process Waste Support
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project
+ SR-HL01	C-249	H-Tank Farm
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations

Environmental Management Science Program Research in Washington

Pacific Northwest National Laboratory

54684-WA - Mechanism Involved in Trichloroethylene-Induced Liver Cancer: Importance to Environmental Cleanup

Year of Award: 1996 **Amount of Award:** $1,800,000
Problem Area: Health / Ecology / Risk
Science Category/SubCategory: Health Science / Health Effects
Principal Investigator: Dr. Richard J. Bull, 509-373-6218, rj_bull@ccmail.pnl.gov
Major Collaborator(s): Richard Okita at Washington State University
For More Information: http://www.doe.gov/em52/54684.html

Description Provided by Investigator:

Clean-up costs for chlorinated solvents found on DOE sites are most frequently driven by trichloroethylene (TCE). More permissive standards for TCE would reduce DOE's complex-wide clean up costs by several billions of dollars. EPA is currently reviewing its risk assessment for TCE. The research proposed will provide direct input into that process from three interrelated projects: 1) To determine whether selection rather than mutation accounts for the TCE-induced shift in H-ras mutation spectra in tumors. Dose-response information necessary for risk-based standards must be developed *in vivo.* 2) To seek direct evidence for the selection mechanism *in vitro.* This will provide direct evidence of a non-genotoxic mechanism and is essential for selection of a non-linear extrapolation model for estimating risk at low exposures. The default model is linear, based on genotoxic mechanisms. 3) To determine the importance of the peroxisome proliferation activated receptor (PPAR) to TCE-induction of liver tumors as an alternative non-genotoxic mechanism. This would also justify use of a non-linear extrapolation model. If either mechanism is shown responsible for liver tumors induced by TCE, liver tumor induction will not be the most sensitive parameter for establishing clean-up standards. Thus, risk-based clean-up standards could increase by an order of magnitude.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Health / Ecology / Risk problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Health / Ecology / Risk".

Environmental Management Science Program Research in Washington

Pacific Northwest National Laboratory

54996-WA - Ionizing Radiation Induced Catalysis on Metal Oxide Particles

Year of Award: 1996 **Amount of Award:** $1,110,000
Problem Area: High Level Waste
Science Category/SubCategory: Separations Chemistry / Catalyst Chemistry and Waste Treatment
Principal Investigator: Dr. Teresa Fryberger, 509-376-6688, t_fryberger@ccmail.pnl.gov
For More Information: http://www.doe.gov/em52/54996.html

Description Provided by Investigator:

This reseach investigates a novel approach for destroying organics, such as those found in a variety of DOE waste and process streams. We propose that organics can be destroyed utilizing redox chemistry resulting from electron-hole (e^-/h^+) pairs generated in stable, wide bandgap semiconductors via interactions with ionizing radiation (α, γ, γ). Conceptually this process is an extension of visible and near-UV photocatalytic processes known to occur at the interfaces of narrow bandgap semiconductors in both solution and gas phases, and which have been shown, for example, to completely oxidize chlorinated hydrocarbons to CO_2 and HCl without hydrogen gas emission. The advantages of using heterogeneous catalysis to destroy organics found in wastes is that 1)it is emission free and 2) it does not require elevated temperatures or pressures--a drawback of many other destruction technologies. Further advantages of using ionizing radiation include 1) it overcomes optical transparency limitations associated with visible and near-UV illumination (thus processing would not require optical windows and could be done directly in a waste stream) and 2) it permits the use of wider bandgap materials (such as ZrO_2) that possess potentially greater redox capabilities than materials with narrow bandgaps. The extension to wider bandgap materials will broaden the range of accessible organic destruction reactions, and potentially extend the process to reductive metal and metal oxide deposition. We have demonstrated the validity of this extension for the destruction of a typical organic species present in tank waste on the Hanford site (ethylene diamine tetraacetic acid - EDTA) using γ radiation from ^{60}Co source to generate e^-/h^+ pairs in TiO_2 based catalysts.

As a means of furthering this concept of using ionizing radiation to perform e^-/h^+ chemistry on semiconductor catalysts, we are conducting experiments aimed at 1) expanding the body of knowledge about e^-/h^+ pair chemistry of semiconducting metal oxide (MO) materials by examining and comparing the photocatalytic and radiocatalytic behavior of a well-studied narrow bandgap material,TiO_2, and 2) extending these studies to wider bandgap materials (ZrO_2) that are virtually unexplored in terms of their e^-/h^+ pair chemistry. An outcome of this work will be a more thorough evaluation of the use of ionizing radiation in the catalytic remediation of organics in high-level mixed waste. Ultimately, the goal of this work will be to develop the predictive capability required to apply this approach for the treatment of a broad spectrum of both DOE and industrial wastes and process streams. Gamma irradiation sources ranging from industiral Co-60 sources to Cs-137 capsules at the Hanford site could be used to provide the ionizing radiation in this concept.

The radiocatalysis concept satisfies a number of direct needs from the EMSP call for proposals: 1) emission-free destruction of organic wastes, 2) nonthermal treatment concepts for mixed waste, and 3) pretreatment and separation methods that lead to a significant reduction in the amount of immobilized high-level waste requiring long-term isolation. Additionally, this work will provide a better understanding of radiation-induced interfacial reactions at oxides existing in the tank waste and is complementary to ongoing work in another EMSP project--"Radiolysis Effects in Tank Waste Speciation " (T. Orlando, PNNL).

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§ SR-HL05	C-265	Vitrification
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project
+ SR-SW01	C-281	Consolidated Incinerator Facility
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in Washington

Pacific Northwest National Laboratory

55031-WA - Genetic Analysis of Stress Responses in Soil Bacteria for Enhanced Bioremediation of Mixed Contaminants

Year of Award: 1996 **Amount of Award:** $1,021,886
Problem Area: Remedial Action
Science Category/SubCategory: Microbial Science / Microbial Genetics and Instrumentation
Principal Investigator: Dr. Kwong-Kwok Wong, 509-376-5097
Major Collaborator(s): Ronald Olsen at the University of Michigan
For More Information: http://www.doe.gov/em52/55031.html

Description Provided by Investigator:

Bioremediation is, in some cases, a cost-effective approach to site clean-up. However, to realize the full potential of this biological process, fundamental information is needed about genetic responses of bacteria to environmental factors in the contaminated subsurface. Identification of changes in gene expression that result from *in situ* stresses - primarily low nutrients, low oxygen, and organic solvents-will provide basic information relevant to bioremediation strategies.

We will identify the stress-inducible genes from two soil bacteria, *Deinococcus radiodurans and Sphingomonas F199.* These organisms represent two phylogenetically distinct groups of soil bacteria, each of which has specific features of interest for bioremediation. *D. radiodurans* exhibits high resistance to external stress; F199 is a deep subsurface (Savannah River Site) organism with unique degradative capabilities. The resulting fundamental information on stress-responsive genes will provide an increased knowledge of stress responses of indigenous microbes at contaminated sites as well as molecular probes for monitoring performance and effectiveness of bioremediation. We will also evaluate the use of identified stress responsive genes to direct the expression of toluene monooxygenase cloned from Burkholderia pickettii into Deinococcus radiodurans for effective trichloroethylene (TCE) degradation.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§ RL-ER08	C-147	Groundwater Management
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Washington

Pacific Northwest National Laboratory

60345-WA - New Silicotitanate Waste Forms: Development and Characterization

Year of Award: 1997 **Amount of Award:** $1,200,000
Problem Area: High Level Waste
Science Category/SubCategory: Materials Science / Chemical and Structural Properties Of Storage Materials
Principal Investigator: Dr. Mari Lou Balmer, 509-372-4693, ml_balmer@pnl.gov
Major Collaborator(s): Dr. Tina Nenoff at Sandia National Laboratories - Albuquerque
Dr. Alexandria Navrotsky at the University of California at Davis
For More Information: http://www.doe.gov/em52/60345.html

Description Provided by Investigator:

The program outlines a new strategy for disposing of crystalline silicotitanate (CST) ion exchangers by in-situ heat treatment to produce an alternate waste form. New waste forms and disposal strategies specific to CST secondary waste that are developed in this work will offer an alternative to current disposal plans which call for recombining the separated Cs, Sr-loaded CST into the high activity waste streams then dissolving it in borosilicate glass. This research is predicated by work at Pacific Northwest National Laboratory that shows that thermally treated CSTs have durabilities better than borosilicate glass. The goal of the program is to reduce the costs associated with CST waste disposal, to minimize the risk of contamination to the environment during CST processing, and to provide DOE with technical alternatives for CST disposal. Because there is uncertainty in repository availability and in waste acceptance criteria, it is likely that Cs and Sr loaded ion exchangers will require short term storage at Hanford or that new scenarios for long term storage or disposal of nuclides with relatively short half lives (such as ^{137}Cs and ^{90}Sr) will arise.

Continuing the initial CST materials research from Sandia, the research will synthetically explore both low and high temperature stable and metastable phases involving the key component elements. This will allow for characterization (ie., kinetic studies at UC Davis) of all potential by-products from thermal treatment of CSTs. The resulting work will provide information on the durabilities and stabilities of thermally consolidated CSTs so that the potential of these options as viable storage or disposal scenarios can be evaluated. The technical objective of the work is to (1) fully characterize the phase relationships, structures and thermodynamic and kinetic stabilities of crystalline silocotitanate waste forms, and (2) to establish a sound technical basis for understanding key waste form properties, such as melting temperatures and aqueous durability, based on an in-depth understanding of waste form structures and thermochemistry

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§ ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§+ RL-TW08	C-185	Process Waste Privatization Infrastructure
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§ SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Washington

Pacific Northwest National Laboratory

60355-WA - Mineral Surface Processes Responsible for the Decreased Retardation (or Enhanced Mobilization) of 137Cs from HLW Tank Discharges

Year of Award: 1997 **Amount of Award:** $1,250,000
Problem Area: Remedial Action
Science Category/SubCategory: Geochemistry / Sorption/Desorption
Principal Investigator: Dr. John M. Zachara, 509-375-2993, jm_zachara@pnl.gov
Major Collaborator(s): Dr. Paul M. Bertsch at Savannah River Ecology Laboratory
For More Information: http://www.doe.gov/em52/60355.html

Description Provided by Investigator:

High level wastes (HLW) were generated during the extraction of Pu and other elements from irradiated uranium fuels. Most of the HLW remain stored at the Hanford site in 177 massive underground storage tanks. Sixty-seven of these tanks have leaked discharging ca. 1 million gallons of waste to the subsurface containing 1 million Ci of radiation, most of which is ^{137}Cs. Although strongly sorbed by the micaceous fraction of the underlying sediments, ^{137}Cs$^+$ has migrated significant distances below some tanks leading to concern that it may reach groundwater.

This project will investigate the geochemistry of Cs$^+$ adsorption under conditions relevant to HLW tank releases. Emphasis is placed on Hanford REDOX wastes, as field evidence suggests that the chemical composition of these promote enhanced subsurface Cs migration. The central research tenets are that the high Na concentrations in the HLW will suppress all but the most selective Cs sorption sites that occur on the frayed edges of micaceous particles (FES), and that FES may be chemically altered by hydroxide and aluminate in HLW.

The research integrates studies of ion exchange thermodynamics on the FES, with high resolution surface microscopies (HRTEM, AFM, TOF-SIMMS) and molecular spectroscopy (NMR, EXAFS) to probe the structure of FES in Hanford sediments and how the chemical environment of sorbed Cs changes when HLW supernatants promote sorbent dissolution and the precipitation of new phases. Our goal is to develop field relevant knowledge to improve transport calculations of Cs beneath the tank farms and provide needed insights for long term decision making pertaining to performance/risk assessment and site-restoration. Specifically, the research will:

- Identify how the macroscopic sorption behavior of Cs on the micaceous fraction of Hanford sediments changes after contact with HLW simulants as a function of temperature and chemical parameters.
- Reconcile observed changes in Cs sorption chemistry with microscopic and molecular changes in the site distribution, chemistry, mineralogy, and morphology/structure of highly selective sorption sites in the micaceous fraction.
- Integrate mass action solution exchange measurements with microscopic characterization of the surface structure and chemistry of the selective sorbent phase to yield a multi-component exchange model for prediction of Cs sorption.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ AL007	C-7	Environmental Restoration
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§ NV212	C-49	Underground Test Area (UGTA)
§ NV214	C-53	Industrial Sites
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§+ RL-ER01	C-125	100 Area Remedial Action
§+ RL-ER03	C-133	300 Area Remedial Action
§ SR-ER03	C-223	Lower Three Runs & Operations Project
§+ SR-ER06	C-227	Upper Three Runs Project
+ RL-TW04	C-169	Retrieval Project
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
+ SR-HL02	C-253	F-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations

Environmental Management Science Program Research in Washington

Pacific Northwest National Laboratory

60362-WA - Ion-Exchange Processes and Mechanisms in Glasses

Year of Award: 1997 **Amount of Award:** $901,000
Problem Area: High Level Waste
Science Category/SubCategory: Materials Science / Chemical and Structural Properties Of Storage Materials
Principal Investigator: Dr. B. Peter McGrail, 509-376-9193, Pete.McGrail@pnl.gov
Major Collaborator(s): Dr. David K. Shuh at Lawrence Berkeley National Laboratory
For More Information: http://www.doe.gov/em52/60362.html

Description Provided by Investigator:

Recent performance assessment calculations of a disposal system at Hanford, Washington for low activity waste glass show that a Na ion-exchange reaction can effectively increase the radionuclide release rate by over a factor of 1000 and so is a major factor that currently limits waste loading. However, low temperature ion exchange has not been thought to be important in recent analyses of waste glass durability. The objective of this work is to develop an understanding of the processes and mechanisms controlling alkali ion exchange and to correlate the kinetics of the ion-exchange reaction with glass structural properties.

Ion-exchange reaction mechanisms will be studied by using nuclear reaction analysis techniques to probe the distribution of isotopically-labeled elements in the hydrated layers on glass surfaces. Differences in the uptake and distribution of these isotopes will provide a signature characteristic of specific ion-exchange reactions. X-ray absorption spectroscopy will be used to identify and correlate key structural properties, such as the number of nonbridging oxygens, bonding of alkali to other elements in the glass, and alkali coordination, with differences in measured rates of alkali exchange. The fundamental understanding of the ion-exchange process developed under this study will provide a sound scientific basis for formulating low exchange rate glasses with higher waste loading, resulting in substantial production and disposal cost savings.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§ ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
§+ RL-TW04	C-169	Retrieval Project
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ RL-TW08	C-185	Process Waste Privatization Infrastructure
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
§ SR-HL05	C-265	Vitrification
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in Washington

Pacific Northwest National Laboratory

60387-WA - Distribution & Solubility of Radionuclides & Neutron Absorbers in Waste Forms for Disposition of Plutonium Ash & Scraps, Excess Plutonium, and Miscellaneous Spent Nuclear Fuels

Year of Award: 1997 **Amount of Award:** $1,800,000
Problem Area: Nuclear Materials
Science Category/SubCategory: Materials Science / Chemical and Structural Properties Of Storage Materials
Principal Investigator: Dr. Xiangdong Feng, 509-373-7284, X_Feng@ccmail.pnl.gov
Major Collaborator(s): Dr. Eric R. Vance at Australian Nuclear Science & Technology Organisation
Dr. David K. Shuh at Lawrence Berkeley National Laboratory
Dr. Rodney C. Ewing at the University of Michigan
For More Information: http://www.doe.gov/em52/60387.html

Description Provided by Investigator:

The objective of this multi-institutional, multi-national research effort is to understand the distributions, solubilities, and releases of radionuclides and neutron absorbers in waste forms. The results will provide the underpinning knowledge for developing, evaluating, selecting, and matching waste forms for the safe disposal of various wastes associated with Pu, miscellaneous spent nuclear fuels (SNF), and other transuranic (TRU) wastes and for developing deterministic model for the long-term performance assessment of radionuclide containment.

The scope of this project includes: 1) systematically investigate the solubility and partition behavior of selected waste forms as a function of composition, temperature, and processing conditions with the goal of enhancing our understanding of the physics and chemistry of radionuclides and neutron absorbers in simplified waste forms; 2) determine the local structure of radionuclides and neutron absorbers waste forms in various phases: a) a microscale characterization to determine what phases are presented and how key elements are partitioned among those phases using optical, scanning, and transmission microscopies and XRD; b) a molecular level characterization to understand local coordination using EXAFS and NMR; c) an atomic level characterization to determine oxidation state using XANES; 3) selectively study waste form properties with the emphasis on the release behaviors of neutron absorbers and radionuclides.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Nuclear Materials problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Nuclear Materials".

Environmental Management Science Program Research in Washington

Pacific Northwest National Laboratory

60392-WA - Radiolytic and Thermal Process Relevant to Dry Storage of Spent Nuclear Fuels

Year of Award: 1997 **Amount of Award:** $891,000
Problem Area: Spent Nuclear Fuel
Science Category/SubCategory: Separations Chemistry / Catalyst Chemistry and Waste Treatment
Principal Investigator: Dr. Steven C. Marschman, 509-376-3569, steve.marschman@pnl.gov
Major Collaborator(s): Dr. Peter E. Haustein at Brookhaven National Laboratory
Dr. Theodore E. Madey at the Rutgers, the State University of New Jersey
For More Information: http://www.doe.gov/em52/60392.html

Description Provided by Investigator:

Thousands of tons of metallic uranium spent-nuclear-fuel (SNF) remain in water storage across the Department of Energy complex. For example, the Hanford Site K-Basins hold 2300 metric tons of spent fuel, much of it severely corroded. Similar situations exist elsewhere in the DOE complex, especially at Savannah River and Idaho National Engineering and Environmental Laboratory. The DOE plans to remove much of this fuel and seal it in canisters for "dry" interim storage, for up to 75 years awaiting permanent disposition. Chemically-bound water will remain in cracks and bound to surfaces even following proposed drying steps, leading to possible long-term corrosion of the containers and/or fuel rods themselves, generation of H_2 and O_2 gas via radiolysis which could lead to deflagration or detonation, and reactions of pyrophoric uranium hybrides. No thoroughly tested model is currently available to predict fuel behavior during pre-processing, processing, or storage. We propose to study the radiolytic reactions, "drying" processes, and corrosion behavior of actual SNF materials, and of pure and mixed-phase samples, to determine what is omitted from current models: radiolysis of water adsorbed on or in hydrates or hydroxides, thermodynamics of interfacial phases, and kinetics of drying. A model will be developed and tested against actual fuel rod behavior to insure validity and applicability to the problems associated with developing dry storage strategies for DOE-owned SNF.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Spent Nuclear Fuel problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Spent Nuclear Fuel".

Environmental Management Science Program Research in Washington

Pacific Northwest National Laboratory

60451-WA - Mechanics of Bubbles in Sludges and Slurries

Year of Award: 1997 **Amount of Award:** $1,132,000
Problem Area: High Level Waste
Science Category/SubCategory: Engineering Science / Bubble Mechanics and Sonification
Principal Investigator: Dr. Phillip A. Gauglitz, 509-372-1210, pa_gauglitz@pnl.gov
Major Collaborator(s): Dr. Morton M. Denn at Lawrence Berkeley National Laboratory
Dr. William R. Rossen at the University of Texas at Austin
For More Information: http://www.doe.gov/em52/60451.html

Description Provided by Investigator:

Previous studies have established that the waste level of Hanford tanks responds to barometric pressure changes, the compressibility of retained bubbles accounts for the level changes, and the volume of retained gas can be determined from the measured waste level and barometric pressure changes. However, interactions between the gas bubbles and rheologically complex waste cause inaccurate retained gas estimates and are not well understood. Because the retained gas is typically a flammable mixture of hydrogen, ammonia, and nitrous oxide, accurate determination of the retained gas volume is a critical component for establishing the safety hazard of the tanks. Accurate estimates of retained gas from level/pressure data are highly desirable because direct in situ measurements are very expensive in an individual tank and impossible in many single-shell tanks.

The objective of the research is to gain a fundamental understanding of the interactions between gas bubbles and tank waste during barometric pressure fluctuations. This understanding will have a direct influence on improving the accuracy of gas volume estimates for Hanford tanks from the nonintrusive level and pressure measurements. The elucidation of the bubble waste interactions should also provide more accurate models for estimating waste properties from level/pressure data and should quantify the effect of barometric pressure fluctuations on the slow release of bubbles.

The proposed studies will be tackled by a team with complementary areas of expertise that pertain directly to the central issues. The core team has expertise on bubble behavior in Hanford waste (Gauglitz), expertise on Hanford waste rheological properties and solid mechanics (Terrones), a wealth of experience on modeling and characterizing complex fluids (Denn and Muller), and expertise on modeling movement and capillary effects in porous media (Rossen).

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the <u>Index of High Cost Environmental Management Projects by Problem Area</u>, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment

Environmental Management Science Program Research in Washington

University of Washington

54800-WA - Construction of Bending Magnet Beamline at the APS for Environmental Studies

Year of Award: 1996 **Amount of Award:** $810,000
Problem Area: Remedial Action
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Sensors and Techniques
Principal Investigator: Dr. Edward A. Stern, 206-543-2023, stern@phys.washington.edu
For More Information: http://www.doe.gov/em52/54800.html

Description Provided by Investigator:

Introduction

Synchrotron radiation studies of materials at the molecular scale can make important contributions to the understanding of the basic science issues underlying environmental cleanup efforts. A recent DOE workshop report "Molecular Environmental Science: Speciation, Reactivity, and Mobility of Environmental Contaminants" (July 5-8, 1995) emphasizes the important role to be played by synchrotron techniques, especially in the hard x-ray range. This view is confirmed by the increasing numbers of environmental programs which are employing synchrotron techniques, and the report also concludes that the available beamtime for such experiments is likely to be saturated in the near future. It is equally important that the beamtime be accompanied by the appropriate support for environmental studies, such as the capabilities for handling radioactive samples. To address these issues the Pacific Northwest Consortium-Collaborative Access Team (PNC-CAT) is proposing to build the optics and beam transport of a bending magnet beamline to deliver x-rays to an experimental enclosure. The beamline will be located at sector 20 of the Advanced Photon Source (APS), and will share important environmental support facilities with an insertion device beamline already under construction.

The PNC-CAT is a consortium of researchers from Universities in Washington State, Canada, and the Pacific Northwest National Laboratory (PNNL) in Richland, Washington. The PNC-CAT was formed to develop a sector at the Advanced Photon Source (APS), a third-generation synchrotron radiation x-ray source under construction at Argonne National Laboratory. This source will be completed in 1996-1997, and its distinguishing feature will be the use of insertion devices such as undulators which increase source brightness by orders of magnitude over previous generation synchrotrons. The PNC-CAT will employ this source brilliance to develop a unique x-ray microbeam of unprecedented flux density with beam size and resolution down to ~0.1 micron, and tunable over the range 4-25 keV for a variety of research projects. Equipped with an x-ray microprobe, advanced fluorescence detectors, radioactive sample facilities, and surface scattering and XAFS equipment, the PNC-CAT beamlines provide unique facilities for basic research into environmental problems.

The University of Washington (UW) has recently recognized its special responsibility because of its geographic location, to help in solving the clean-up problems at the badly contaminated Hanford, Washington, site. The University Administration has been encouraging Faculty involvement in this activity (see Letter in Appendix A). In particular, as stated in the Letter, "The University of Washington will match all awards received through the EMSP program at the level of 10%." The facilities in this research will not only give unique capabilities to investigate the research problems proposed here, but also will be of use to the programs of other researchers, including collaboration with researchers from UW and PNNL as outlined in Section D. For example, a number of ongoing Environmental Management (EM) problems will be addressed by the basic research planned for the beamlines. These include:

- Improved waste processing and separation technologies.
- Alternative waste forms capable of better handling of problematic species such as Ti or phosphates.
- Verification of modeling for the transport of contaminants under geologic conditions.
- Chemical speciation of tank wastes.

- Atomic scale structure of active sites in metallo-enzymes proposed for bio-catalytic reduction of actinides, metal contaminants and chlorinated hydrocarbons.

- Adsorption and catalytic interactions at mineral surfaces.

- Radiation induced structural changes in waste forms.

- Improved sensors for monitoring contaminants.

The estimated number of key personnel who will be utilizing this instrumentation consists of the following: senior personnel, 37; post-docs, 10; graduate students, 20; and undergraduates, 5. The members of the PNC-CAT cover a broad spectrum of interest. All are interested in the fundamental properties of "materials" but differ in the materials being investigated and the areas of application of this basic knowledge. The unifying element is the PNC-CAT and the experimental capabilities that its facilities will present. As has been the experience at other synchrotron sources, the PNC-CAT is expected to catalyze interactions between governmental and industrial researchers, graduate students, professors and post-docs from different fields which would not have occurred otherwise.

Project Summary

To help satisfy the growing need for synchrotron radiation based environmental research, it is proposed to carry out the design and construction of a bending magnet (BM) beamline at the Advanced Photon Source (APS) by the Pacific Northwest Consortium-Collaborative Access Team (PNC-CAT). The line will be optimized for various forms of x-ray absorption spectroscopies (XAS). Environmental and cleanup issues are a major focus of the fundamental research to be performed on the BM beamline. The beamline will share the PNC-CAT experimental facilities to be fabricated for the neighboring Undulator A Insertion Device beamline to utilize the experimental techniques of x-ray absorption spectroscopy for both bulk and surface studies, with spatial and time resolution and elemental imaging, on toxic and radioactive samples. These capabilities have been cited in a recent DOE workshop report as most desirable for future environmental research.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

Environmental Management Science Program Research in Washington

University of Washington

54889-WA - Using Trees to Remediate Groundwaters Contaminated with Chlorinated Hydrocarbons

Year of Award: 1996 **Amount of Award:** $650,578
Problem Area: Remedial Action
Science Category/SubCategory: Plant Science / Plant Metabolism
Principal Investigator: Dr. Stuart E. Strand, 206-543-5350, sstrand@saul.u.washington.edu
For More Information: http://www.doe.gov/em52/54889.html

Description Provided by Investigator:

Phytoremediation has emerged as a treatment alternative that combines the low cost of intrinsic remediation with the more active and adaptable characteristics of conventional remediation. Our lab has shown that fast-growing and deep-rooted hybrid poplar take up and transpire trichloroethylene (TCE) at a high rate, and that significant amounts of TCE are oxidized to carbon dioxide. These findings have been confirmed with axenic tissue cultures and with unique laboratory bioreactors that provide complete mass balance accounting of the fate of TCE carbon with whole plants. Ongoing field trials of small plots of poplar exposed to TCE have provided striking confirmation of the ability of these trees to completely prevent the movement of TCE through a barrier of densely planted poplar. We have also made significant progress in iden tifying the mechanism of TCE degradation in poplar (cytochrome P-450 IIE 1) and in constructing transgenic plants with enhanced capability for degradation of chlorinated hydrocarbons (CHCs). Finally recent evidence suggests that poplar will also be capable of uptake and oxidation of carbon tetrachloride.

We propose to test the ability of several plant clones to take up and transform various CHCs, including carbon tetrachloride, chloroform, dichloromethane, 1,1,1-trichloroethane, perchloroethylene, trichloroethylene, the dichloroethylenes, and vinyl chloride using laboratory mass balance reactors. Screening methods have been developed that permit testing of plants from contaminated sites for those able to oxidize and sequester chlorinated compounds. In order to predict the best location and size of the plantation and hydrogeological models will be developed which include uptake of water and pollutants from the aquifer by trees. We will identify the mechanisms involved in CHC oxidation in poplar. We enhance that activity by amplifying expression of native monooxygenases or mammalian P-450s in poplar.

We anticipate that these approaches will provide powerful new tools for the remediation arsenal: selfmaintaining, solar-driven, pump-and-treat systems.

Background and Significance

Industrial practices in the past have resulted in contamination of groundwater with chlorinated hydrocarbons (CHCs) at many DOE sites, such as Hanford and Savannah River. Such contamination is a major problem because existing groundwater remediation technologies are expensive and difficult. An inexpensive method for groundwater remediation is greatly needed.

An alternative to costly conventional technologies is intrinsic remediation, which uses natural processes intrinsic to some polluted groundwaters that result in degradation, dilution or immobilization of the pollutant before adverse health effects can occur. Unfortunately not all sites have the requisite conditions to permit intrinsic remediation to occur at a rate which make it a viable option. Frequently, it is unclear whether there is sufficient electron donor present to maintain the requisite anaerobic conditions to sustain intrinsic remediation of CHCs for the timerequired to treat all of the pollutant that may be present. Furthermore, intrinsic remediation relies on natural groundwater flow to flush the polluted aquifer clean, extending the time required forcleanup.

Recently another option has emerged that combines the minimal intervention and costs of intrinsic remediation with the more active and adaptable characteristics of conventional remediation approaches. This option is phytoremediation and the University of Washington has taken a leading role in its application to groundwaters polluted with CHCs. Phytoremediation is the use of plants to clean up contaminated soil, water and air.

Trees could be used to provide an active remediation zone and barrier to pollutant movement at minimal cost. Cost analysis suggests that phytoremediation would cost less than half the cost of conventional pump-and-strip technology over the 30-year life of the project. Since most of the cost of phytoremediation would be due to monitoring requirements, this outlay would be comparable to that required for intrinsic remediation. Poplar wood is valuable as a source of chips for paper making and its sale would partially offset the cost of phytoremediation. Poplar grow rapidly, reaching 30 m in nine years. Their roots seek out water from depths up to 20 m. Their transpiration rate is very high and their ability to prevent the movement of nitrate contaminated water off agricultural sites has been well demonstrated. Approximately 80% of the CHC polluted aquifers in the US are within 20 m of the surface, thus potentially accessible to poplar roots.

Poplar could be used to assist in the clean up of the contaminated groundwater at Hanford with beneficial effects on the major mobile pollutants: nitrate, carbon tetrachloride and tritium. A phytoremediation barrier could be established across the contaminated plume as it approaches the Columbia River. Near the river the plume is shallow enough for trees to access the groundwater. A sufficiently large plantation of densely planted poplar could prevent the plume from reaching the river. These trees would easily take up and assimilate the nitrate. Tritium contaminated water would be assimilated into plant tissue and transpired to the atmosphere, where sufficient dilution exists to prevent serious harm. Carbon tetrachloride would be transpired, metabolized and sequestered in plant tissue, and oxidized to carbon dioxide, depending on the trees planted. Over the lifetime of the plantation (50 years or more) trees would be harvested, sold for pulp, and new trees would be planted. A poplar plantation barrier would be much less expensive than other active remediation technologies.

Before phytoremediation can be extensively applied, we must determine the range of compounds that are attacked, the effects of metabolic products on the plants and the environment, and the effect of transpiration and concentration of CHC on uptake and metabolism. Aside from TCE very little is known of what other CHCs can be transported and/or oxidized by plants. A survey should be made of the CHC degradation ability of trees adapted to growth in various locales so that phytoremediation can be applied across the country. Little is known about the distribution of CHC degradation capability in plants. These capabilities should be surveyed by testing a wide variety of plants. Trees already growing on contaminated sites should be tested to determine if they have adapted by metabolizing the pollutants. Hydrogeological models that include the effects of trees on groundwaters polluted with CHCs are needed to provide rules for designing phytoremediation plantations. In order to capitalize on the promise of phytoremediation as illus trated by our findings of TCE metabolites in poplar tissue, we need to understand the mechanisms of plant metabolism of TCE and to explore transgenic mechanisms for increasing TCE degradation.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§ RL-ER08	C-147	Groundwater Management
§+ SR-ER06	C-227	Upper Three Runs Project

Environmental Management Science Program Research in Washington

University of Washington

54897-WA - The Sonophysics and Sonochemistry of Liquid Waste Quantification and Remediation

Year of Award: 1996 **Amount of Award:** $769,843
Problem Area: Mixed Waste
Science Category/SubCategory: Inorganic Chemistry / Multiphase/Gaseous Chemistry
Principal Investigator: Dr. Thomas J. Matula, 206-543-1300, matula@crosby.apl.washington.edu
For More Information: http://www.doe.gov/em52/54897.html

Description Provided by Investigator:

Some Background

When an ultrasonic field of moderate to large intensity is applied to a liquid, the liquid often fails under the action of the dynamic tensile stress applied by the ultrasound. Consequently, the vapor cavity that is formed during the rarefaction portion of the sound field can thus grow rapidly so long as the applied negative acoustic pressure exceeds the vapor pressure of the liquid; subsequently, however, this cavity is driven into an implosive collapse as the sound field turns positive and applies a compressive force to the cavity. Because of surface tension, the cavity remains spherical for much of its life cycle and, accordingly, an enormous energy concentration--as much as 12 orders of magnitude--can result from this growth and collapse sequence--a phenomenon called acoustic cavitation. The temperatures and pressures experienced by the material contained within the imploding cavities can achieve values in excess of tens of thousands of degrees and tens of kilobars, respectively. These high temperatures and pressures can act as an intense microreactor and induce a variety of chemical reactions; the ability of these reactions to induce a particular effect is called sonochemistry, and holds high promise as a specific chemical approach to waste contaminant remediation.

The Promise

A variety of investigators have demonstrated the utility of the sonochemical reactor; for example, the natural half-life of parathion, a pesticide of widespread use, is 108 days. Under ultrasonic irradiation at 20 kHz in deionized water, all of the initial parathion is degraded in less than two hours; ultrasonic irradiation in an aqueous solution containing the highly toxic pentachlorophenate (PCP) results in the almost complete degradation of PCP in about 100 minutes; researchers have also found that acoustic irradiation of chlorinated C1 and C2 volatile organic compounds (VOCs) resulted in a VOC destruction of up to 99.9% in less than an hour.

The Problem

Although sonochemistry holds such high promise for use in waste contaminant remediation, the principal mechanism that leads to chemical degradation, acoustic cavitation, is a complex and difficult to understand phenomenon. Chemists who are performing experiments in sonochemistry know little of acoustic cavitation and how to use it in an optimal way; physicists who know something about cavitation bubble dynamics don't understand the chemistry. Indeed, the President of the European Society of Sonochemistry has deemed this field a "black art", whose progress is mainly empirical, and which will lack credibility as a mature science until multidisciplinary teams involving both physicists and chemists examine the problem from a fundamental viewpoint. We propose a systematic study of the phenomenon of acoustic cavitation as it applies to sonochemistry, and especially as it applies to waste contaminant remediation.

The Team

We have established a multidisciplinary team involving internationally recognized experts in the field of acoustic cavitation from the Applied Physics Laboratory at the University of Washington; they will be joined by experts in the field of industrial/analytical chemistry from the Center for Process Analytic Chemistry, also at the University of Washington; participating as consultants are recognized experts from Lawrence Livermore National Laboratory, Savannah River Technology Center, Pacific Northwest National Laboratory, and the University of California, Irvine.

Finally, the University of Washington itself plans an extensive and comprehensive research program in this general area.

The Research Plan

We propose an in-depth and comprehensive study of the fundamentals of acoustic cavitation and nonlinear bubble dynamics, to elucidate the fundamental physics of sonochemical reactions, to examine the potential of sonoluminescence to quantify and to monitor the presence of alkali metals and other elements in waste liquids, to design and to evaluate more effective sonochemical reactors, and to determine the optimal acoustical parameters in the use of sonochemistry for liquid-waste-contaminant remediation.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW03	C-287	Mixed Low Level Waste Project
+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
OR-43204	C-77	ORNL Bethel Valley Deactivation and Decommissioning
+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ OR-46301	C-107	Portsmouth Remedial Action
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
RL-ER08	C-147	Groundwater Management
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW04	C-169	Retrieval Project
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project
+ SR-HL01	C-249	H-Tank Farm
+ SR-HL02	C-253	F-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Washington

University of Washington

55146-WA - Adsorption/Membrane Filtration as a Contaminant Concentration and Separation Process for Mixed Wastes and Tank Wastes

Year of Award: 1996 **Amount of Award:** $609,987
Problem Area: Mixed Waste
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Sensors and Techniques
Principal Investigator: Dr. Mark M. Benjamin, 206-543-7645, markbenj@u.washington.edu
For More Information: http://www.doe.gov/em52/55146.html

Description Provided by Investigator:

Overview

The Hanford Reservation is the largest and perhaps most complex Superfund site in the U.S., containing numerous hazardous chemicals and medium- to long-lived radionuclides. Each category of waste presents a different set of scientific and technological challenges for characterization, handling, treatment, storage and disposal. This research is on novel approaches for separating colloidal matter, U, Sr, and Cs from the remaining constituents of the liquid wastes with which they are associated, and from one another.

A wide variety of organic membranes, anion- and cation-exchange resins, other organic adsorbents, solvents and complexing agents have been developed for the treatment of complex, mixed wastes *[IAEA, Advances in technologies, 1994]*. Some of the adsorbents and ion-exchange resins are exceptionally selective and efficient, but they have serious drawbacks that impair their performance when used to treat radioactive wastes. Namely, they are susceptible to thermal, chemical (i.e., oxidative), and radiation-induced degradation, and they are often very expensive. The regeneration of organic media with adsorbed or otherwise retained radionuclides often is incomplete, and, given their chemical instability, their safe disposal is an additional problem.

The major focus of this research is the development of advanced inorganic processes to treat radionuclide-bearing wastes. Inorganic materials are generally much cheaper and less prone to deterioration in radioactive environments than organic materials, their long-term behavior is easier to predict, and they can be used in vitrification processes. However, for inorganic materials to be useful in such applications, significant improvements are needed in their mechanical properties, adsorption and/or exchange capacity, and level of characterization. In this proposal, we explore new processes that employ relatively inexpensive and easy-to-use inorganic materials specifically designed to satisfy the needs of mixed nuclear waste treatment. Another major, novel aspect of this research is the combination of inorganic media with electrochemical methods to enhance, accelerate or create an additional useful control parameter in treatment process.

Proposed Separation Process

Many Hanford wastes contain radionuclides, heavy metals, organic solvents, complexing agents, and inorganic salts (predominantly NaOH and $NaNO_3$)*[Gephardt and Lundrgren; Tank Farm Surveillance, 1993; Chaiko, Vojta, and Takeuchi 1995]*. The sequential treatment system which we propose to develop has as its ultimate goal the separation of contaminants into sub-groups which subsequently can be processed and disposed of appropriately, depending on their properties and the risk they pose. The major emphasis of this research is on the treatment oflow-organic waste. Many of the organic contaminants that might be in the waste are unlikely to interfere with process performance. On the other hand, additional treatment steps might be required to eliminate or deactivate some such species (e.g., complexing agents that are present in significant concentrations).

Research on those portions of an overall treatment process is not included in the proposed effort.

Although the speciation of each contaminant depends on the particular waste being treated, most of the waste is alkaline or neutral *[Gephard and Lundgren]*. Therefore, we anticipate that many of the contaminants of concern (actinides, some other radionuclides, heavy metals) are primarily associated with solids, either as mixed, bulk solids or adsorbed on other particulate matter. The solids range in size from microcolloids to large, settleable particulates. The microcolloids pose major problems for many types of solid/liquid separation systems, since they do not settle easily and can clog filtration systems (either granular media or membrane filters). The first research task will focus on acquiring a more complete understanding of the functioning of an advanced membrane filtration (AMF) system that our group has been developing and that shows promise as an efficient process for removing particulate matter from aqueous wastes. We also propose to study a process developed by other researchers for minimizing fouling of membranes known as electrically enhanced filtration (EEF), and to evaluate a unique combination of these two new technologies.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

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Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW03	C-287	Mixed Low Level Waste Project
ID-HLW-101	C-29	High-Level Waste Pretreatment
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TW04	C-169	Retrieval Project
+ RL-TW05	C-173	Process Waste Support
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
RF014	C-213	Industrial Zone Closure Project
+ SR-HL01	C-249	H-Tank Farm
+ SR-HL02	C-253	F-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Washington

University of Washington

60050-WA - Chemical Speciation of Inorganic Compounds under Hydrothermal Conditions

Year of Award: 1997 **Amount of Award:** $850,000
Problem Area: High Level Waste
Science Category/SubCategory: Separations Chemistry / Catalyst Chemistry and Waste Treatment
Principal Investigator: Dr. Edward A. Stern, 206-543-2023, stern@phys.washington.edu
Major Collaborator(s): Dr. John L. Fulton at Pacific Northwest National Laboratory
For More Information: http://www.doe.gov/em52/60050.html

Description Provided by Investigator:

This research will utilize the high-intensity x-rays available at the Advance Photon Source (APS) to study the inorganic chemistry occurring during the hydrothermal oxidation of tank waste and the chemistry associated with tank waste vitrification. Although the chemical conversion of waste under high-temperature conditions is an integral part of these processing technologies, there is virtually no information in the published literature about the chemical speciation of inorganic compounds under actual processing conditions. This is primarily due to the lack of techniques that are capable of making in-situ measurements of aqueous systems above 300°C. The x-ray-based studies have the unique capability to identify the chemical species and oxidation states of inorganic compounds under extreme solvent conditions. It is imperative to make in situ measurements since the chemical speciation is strongly dependent on temperature. *Thus, the results of this work will provide information critical to the vitrification and hydrothermal oxidation of tank wastes.*

This work is part of a continuing collaborative effort within the Pacific Northwest Consortium Collaborative Access Team (PNC-CAT). The PNC-CAT is a consortium of researchers from the Universities in Washington State, Canada, and the Pacific Northwest National Laboratories (PNNL). This PNC-CAT was formed to develop a sector at the APS, a third-generation synchrotron radiation x-ray source under construction at Argonne National Laboratory. This source is presently in the commissioning stage. Its distinguishing feature is the use of insertion devices such as undulators which increase source brilliance by orders of magnitude over previous generation synchrotrons. The PNC-CAT is employing this source brilliance to develop, among others, a unique x-ray microbeam of unprecendented flux density with beam size and resolution down to 0.1 micron and tunable over the range 4-25 keV for a variety of research projects, including the one proposed here. The PNC-CAT beamlines have the capabilities that have been cited in a recent DOE workshop report ("Molecular Environmental Science: Speciation, Reactivity, and Mobility of Environmental Contaminants" July 5-8, 1995) as most desirable for future environmental research. Our bending magnet beamline is being constructed with the aid of funds allotted by last year's EMSP program

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§ SR-HL05	C-265	Vitrification
AL024	C-3	Grand Junction Office (GJO) All Other Projects
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ OR-48101	C-99	Offsite Remedial Action
+ OR-45301	C-103	Paducah Remedial Action
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER06	C-141	Decontamination and Decommissioning
RL-ER08	C-147	Groundwater Management
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project
+ SR-SW01	C-281	Consolidated Incinerator Facility
+ SR-SW03	C-287	Mixed Low Level Waste Project

Environmental Management Science Program Research in Washington

University of Washington

60123-WA - Potential-Modulated Intercalation of Alkali Cations into Metal Hexacyanoferrate Coated Electrodes

Year of Award: 1997 **Amount of Award:** $300,000
Problem Area: High Level Waste
Science Category/SubCategory: Separations Chemistry / Ligand Design and Ion-exchange
Principal Investigator: Dr. Daniel T. Schwartz, 206-685-4815, Schwartz@cheme.washington.edu
For More Information: http://www.doe.gov/em52/60123.html

Description Provided by Investigator:

The current baseline technology for separating radiocesium (^{137}Cs) from liquid wastes is traditional ion exchange, where chemical regeneration of the ion exchange bed can generate many bed volumes of secondary rinse and regeneration waste solution during each exchange cycle. Chemical regeneration is necessary in traditional ion exchange processes because charge density on the matrix is fixed, leaving the composition of the solution as the main processing variable that can be easily modulated to load or elute ions. Metal hexacyanoferrate (HCF) derivatized electrodes represent a new class of potential-modulated ion exchangers. In these materials, the charge density on the exchange matrix can be modulated using an applied potential (iron-centers in the matrix reversibly switch between the ferrous and ferric states, depending upon the potential). By controlling the charge density on the matrix, ions load or elute in order to maintain charge neutrality within the exchanger, thereby circumventing the need for concentrated chemical regenerants. Derivatized electrodes have been shown to display the same general trends in cation selectivity as bulk HCF exchange materials used in the nuclear power industry. For a potential-modulated ion exchange process , one must use the HCF compound as a thin film (ca. 100 nm) on the electrode because the electronic and ionic conductivity of the matrix is too low to allow redox activity in bulk materials. Past studies of metal HCF derivatized electrodes have focused on the electroanalytical behavior of the interface, and not on the quantitative traits of the derivatized layer that make it well-suited as a potential-modulated ion exchange material.

These studies will explore the effects of fabrication protocol and matrix transport characteristics on the ion exchange capacity, cation selectivity, and cycle-life degradation characteristics of metal HCF derivatized electrodes. The chemistry, electronic properties, and iron-center oxidation state of derivatized layers will be analyzed using *in-situ* imaging Raman spectroscopy and photoelectrochemistry, the ionic selectivity will be analyzed using *ex-situ* electron-based spectroscopies and *in-situ* electrochemical quartz crystal microbalance methods, and the cycle life characteristics will be studied with Raman spectroscopy and the quartz crystal microbalance. Thus, our strategy is to understand and optimize the potential-modulated ion intercalation characteristics of HCF derivatized electrodes through systematic studies of the relationship between materials processing, chemistry, and the resulting properties. In the final stages of the research, insights gained from detailed processing/chemistry/property studies will be combined with methods used in battery technologies to fabricate electrodes with large capacities per unit volume of exchanger.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations

Environmental Management Science Program Research in Washington

University of Washington

60150-WA - Genetic Engineering of a Radiation-Resistant Bacterium for Biodegradation of Mixed Wastes

Year of Award: 1997 **Amount of Award:** $422,398
Problem Area: Mixed Waste
Science Category/SubCategory: Microbial Science / Microbial Genetics and Instrumentation
Principal Investigator: Dr. Mary E. Lidstrom, 206-616-5282, lidstrom@u.washington.edu
For More Information: http://www.doe.gov/em52/60150.html

Description Provided by Investigator:

The mixture of toxic chemicals, heavy metals, halogenated solvents and radionuclides in many DOE waste materials presents a challenging problem for separating the different species and disposing of individual contaminants. One approach for dealing with mixed wastes would be to selectively remove classes of hazardous wastes from mixed waste streams, producing waste streams with less complex mixtures. Because of the initial chemical complexity of such mixtures, these treatment systems should be carried out at relatively low temperatures and pressures and without the addition of new chemicals, to avoid possible secondary reactions that might generate new toxic species. Therefore, a microbiological treatment system is an attractive possibility for separation and treatment. Systems are available in bacteria for detoxifying halogenated organics and toxic metals such as mercury, and theoretically these could be used to selectively remove these classes of compounds from mixed wastes. However, bacteria containing these systems would not be expected to survive in the mixed waste streams that must be treated. Recent work with the deinococci suggests a new approach of gamma-irradiation, and is also highly resistant to desiccation and to peroxides. This resistance is apparently due to highly active DNA repair systems, high chromosome copy number, and an unusual RecA protein. In addition, genetic systems now exist for this organism for cloning, genetic inactivation of chromosomal genes, and expression of foreign genes. Therefore, *D. radiodurans* is a candidate for a strain that could be genetically engineered to survive in and detoxify DOE's mixed waste streams.

In this project, it is proposed to develop a set of *D. radiodurans* strains specifically designed to survive in the toxic conditions found in DOE mixed waste streams. Genes from *E. coli*, *Shigella*, and *phage T4* have been stably expressed in *D. radiodurans*. Therefore, it should be possible to develop expression systems for foreign genes encoding biodegradative functions. In addition, the genome of *D. radiodurans* is currently being sequenced by TIGR, with projected completion and release in 1998. This database will be extremely useful for analyzing expression characteristics of genes and for identifying target genes for future genetic manipulation to increase resistance and optimize expression of foreign genes.

The first goal for this project will be to develop strains that are resistant to a number of toxic metals and that can detoxify a broad range of haloorganics. Specific aims are: 1) develop and optimize expression systems for *D. radiodurans*; 2) clone and express broad spectrum oxygenases that cometabolize haloorganics in *D. radiodurans*; 3) clone and express systems for heavy metal resistance and detoxification in *D. radiodurans*; and 4) test survival and degradation capacity of these strains in artificial mixtures of contaminants, designed to simulate DOE mixed waste streams. Such strains will then be candidates for developing treatment processes for mixed wastes by seeding with dried cells and using non-growth conditions.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
§+ SR-SW01	C-281	Consolidated Incinerator Facility
§+ SR-SW03	C-287	Mixed Low Level Waste Project
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
RF014	C-213	Industrial Zone Closure Project
SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in Washington

Washington State University

60075-WA - Particle Generation by Laser Ablation in Support of Chemical Analysis of High Level Mixed Waste from Plutonium Production Operations

Year of Award: 1997 **Amount of Award:** $544,500
Problem Area: High Level Waste
Science Category/SubCategory: Analytical Chemistry and Instrumentation / Laser Ablation Techniques
Principal Investigator: Dr. J. Thomas Dickinson, 509-335-4914, jtd@wsu.edu
Major Collaborator(s): Dr. Michael L. Alexander at Pacific Northwest National Laboratory
For More Information: http://www.doe.gov/em52/60075.html

Description Provided by Investigator:

Methods for compositional analysis of fissile materials and radioactive/toxic wastes are being developed to support characterization prior to treatment and remediation. The need for rapid, real-time, on site characterization of waste at DOE sites has led to deployment of laser ablation-inductively coupled plasma mass spectroscopy (LA/ICP-MS) systems for elemental and isotopic analysis at several locations, including Hanford, Los Alamos, and INEEL. These systems can provide qualitative or semi-quantitative analysis of certain sample types with minimal sample handling. Research into the fundamental physical processes of particle formation during laser ablation is required to provide basic understanding that will allow us to maximize the utility of these systems. A major consideration is the presence of non-metallic, crystalline and polycrystalline wide bandgap materials or oxide thin films, materials where we have established a breadth of expertise. We propose a collaborative project that combines fundamental studies of mechanisms to provide underlying scientific insight into the relevant parameters influencing productions of particles, the properties of these particles, and relating directly to glove-box installed ICP-MS analysis of both simulants and actual radioactive and toxic waste.

Our work focuses on (1) ablation mechanisms and (2) the effect of the physical and chemical state of the sample (e.g., valance state, impurity concentration, particle morphology, defect concentration, and presence of liquids) on the character of the particles produced by laser ablation. Our goal is to provide physical and chemical insight and useful information for the analytic community to improve prototype instrumentation and analytic techniques for characterizing waste and similar materials. We examine the solid and condensed state properties of the sample, the coupling to the laser beam, and the dynamic electronic, physical, and chemical processes which ultimately generate the particles that are entrained and delivered to a distant ICP unit. This requires careful examination of the intermediate steps such as formation of sub-micron to micron sized particles.

Our research includes studies of the following:

- The absorption mechanisms and the role of laser parameters (wavelength, pulse width, fluence) in coupling energy into the solid.
- Time resolved analysis of the formation of a melt zone, the mechanical response (fracture, shock fronts), and physical ejection of material.
- Careful characterization of the chemical and physical nature of the ejected particles (using several spectroscopies and microscopies).
- The consequences of aggregation and vapor deposition on the particle.
- The role of sample morphology and physical state on particle formation and stoichiometry.
- The influence of liquids (e.g., water, lubricants, solvents) on particle formation and composition.
- The formation mechanisms and morphology and composition of laser produced particles including gas phase aggregation and chemistry.

In general, these studies directly support other analytic methods where lasers are used, e.g., production of plume fluorescence for spectral analysis, vaporization for direct mass analysis, as well as vaporization and particle formation for possible capture by various charged particle traps.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with High Level Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "High Level Waste".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§ ID-HLW-101	C-29	High-Level Waste Pretreatment
§ ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
§+ RL-TW04	C-169	Retrieval Project
§+ RL-TW05	C-173	Process Waste Support
§+ RL-TW06	C-177	Process Waste Privatization Phase I
§+ RL-TW07	C-181	Process Waste Privatization Phase II
§+ RL-TW08	C-185	Process Waste Privatization Infrastructure
§ RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
§+ SR-HL01	C-249	H-Tank Farm
§+ SR-HL02	C-253	F-Tank Farm
§ SR-HL03	C-257	Waste Removal Operations and Tank Closure
§+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
§ SR-HL05	C-265	Vitrification

Environmental Management Science Program Research in West Virginia

West Virginia University

59925-WV - Modeling of Diffusion of Plutonium in Other Metals and of Gaseous Species in Plutonium-Based Systems

Year of Award: 1997 **Amount of Award:** $435,000
Problem Area: Decontamination and Decommissioning
Science Category/SubCategory: Materials Science / Surface Chemistry
Principal Investigator: Dr. Bernard R. Cooper, 304-293-3423, brcoop@wvnvm.wvnet.edu
Major Collaborator(s): Gayanath Fernando at the University of Connecticut
For More Information: http://www.doe.gov/em52/59925.html

Description Provided by Investigator:

The research is aimed at developing and utilizing computational-modeling-based methodology to treat two major problems. The first of these is to be able to predict the diffusion of plutonium from the surface into the interior of another metal such as uranium or stainless steel (fcc iron). The second is the more complicated situation of treating the diffusion of a gaseous species into plutonium-containing oxidized material, specifically the solid-state diffusion of O_2-driven by an oxygen gradient. Consideration of both problems has arisen out of discussion with scientific staff of the Nuclear Materials Technology Division at Los Alamos National Laboratory. The work will proceed in consultation and cooperation with these LANL personnel. The first class of problem, diffusion of plutonium into host metals is pertinent to characterizing contamination and consequent clean-up procedures in situations where plutonium has been in contact with other metals for extended periods of time. The second situation is pertinent to complicated hydrogen generation mechanisms creating possibly catastrophic pressure in situations, such as storage barrels, where oxidized plutonium containing material has been stored for long periods of time.

The enabling aspect of the study is the availability of atomistic potentials of sufficient physical accuracy to capture the nature of the plutonium interactions in the diffusion process. Therefore the availability of physically accurate ab-initio-based atomistic potentials for plutonium, as well as the host iron or uranium metals, is a key and enabling aspect of this study. Among other things, this allows us to treat thermal effects straightforwardly. Because of this key role of the atomistic potentials, initially we will generate these potentials using two different techniques. B. R. Cooper will initially focus on the first of these and G. W. Fernando on the second. We will then select on of the two methods as based on testing of accuracy in comparison to some of our existing fully quantum mechanical calculations and experiment and also, if the two methods provide essentially equally accurate atomistic potentials, as based on computational efficiency. The first method has the strength of our being able to phenomenologically tailor it to include what we perceive to be the key physics of plutonium-based systems, while the second method has the strength of complete objectivity in the information inserted. This second method does, however, depend on inputting the large amount of information needed by use of pseudopotential techniques; and it remains for us to test how well this works for plutonium-based systems.

The two methods for generating interatomic potentials involve: (1) A new technique for constructing many-body atomistic potentials based on ab initio total energy data, starting from a formal expansion of total energy as motivated by Generalized Pseudopotential Theory (GPT). Because of the wide range of deformation energetics included in these calculations, the resulting potentials are expected to provide a more realistic description of materials under large deformation than potentials fitted to physical properties predominantly near equilibrium. (2) Methodology based on the synthesis of a maximum entropy method and total energy calculations; we will generate a large number of configurations with their total energies, as needed for this second method, by the use of plane-wave pseudopotential in Car-Parrinello type dynamics on cells containing a few hundred atoms. The two potential generation methods will be tested in modeling applications by a side-by-side comparison with each other, with ab initio Local Density Approximation (LDA) calculations insofar as possible, and with experiment. These properties will include ones demonstrating transferability of the potentials. We will use the testing and comparison to select one of the two potential generation methods for use in the diffusion calculations. This selection will be on the basis of computational efficiency in generating a potential of comparable physical quality and/or of providing a potential clearly superior in incorporating the physical information. If doubtful of any results, we will always have the option of repeating any calculations using the atomistic potential obtained by the other means.

B. R. Cooper and people working with him at West Virginia University have been actively engaged over the past five years in developing such potentials for *d* transition metals as well as for simple metals. These potentials have been obtained from a data base consisting of full-potential totally energy calculations, using previously developed capabilities for a substantial number of crystallographic configurations. At present, B. R. Cooper, who is a consultant at LANL, is serving as postdoctoral mentor to J. D. Becker, a LANL postdoctoral, who is using *ab initio* force techniques to study lattice relation in supercells containing 32 atoms, e.g. 31 plutoniums and 1 gallium. (This force technique was developed by J. M. Wills of LANL as an outgrowth of the full-potential total energy technique previously developed by J. M. Wills and D. L. Price working with B. R. Cooper at West Virginia University.) The total energies generated at the intermediate and final steps of this procedure, as well as total energies for other lattice configurations will provide the data base used in the first method for extracting the plutonium atomistic potentials.

The investigation of thermally-activated diffusion will make use of transition state theory with dynamic corrections. In transition state theory the number of crossings of a specified counting surface that separates initial and final states is equated to the number of such crossings that occur in an equilibrium system. The use of *ab-initio*-based atomistic potentials will allow us to efficiently map out the pertinent energy barriers. Molecular dynamics can be used to treat realistically the nature of the hoppings as well as to correct for dynamical effects such as recrossings. As guided by experiment, we will use our experience in simulating grain boundaries and incorporating them in dynamic simulations to study the relative importance of grain boundary diffusion in allowing plutonium atoms to penetrate into the interior of the host metals.

Having described the overall nature of the modeling calculations, we will now give further details on the two main components of the modeling study. These are: (1) the treatment of diffusion and of the pertinent grain boundary modeling and (2) the development of physically accurate plutonium atomistic potentials. The physical quality of these potentials is apt to be the controlling quantity in determining the ability to be accurately predictive for the questions of interest.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Decontamination and Decommissioning problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Decontamination and Decommissioning".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
+ OR-48101	C-99	Offsite Remedial Action
+ OR-45301	C-103	Paducah Remedial Action
RL-ER08	C-147	Groundwater Management
+ RL-TP07	C-161	Plutonium Finishing Plant (PFP) Vault Management
+ RL-TW06	C-177	Process Waste Privatization Phase I
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
RF014	C-213	Industrial Zone Closure Project

Environmental Management Science Program Research in British Columbia, Canada

University of British Columbia

54699-CAN-BC - The Use of Dielectric and NMR Measurements to Determine the Pore-Scale Location of Organic Contaminants

Year of Award: 1996 **Amount of Award:** $485,630
Problem Area: Remedial Action
Science Category/SubCategory: Geophysics / Subsurface Imaging
Principal Investigator: Dr. Rosemary Knight, 604-822-3508, knight@geop.ubc.ca
For More Information: http://www.doe.gov/em52/54699.html

Description Provided by Investigator:

A critical step in achieving the cost-effective treatment of a contaminated region of the subsurface is the initial design stage. The design of an effective treatment scheme for a contaminated site requires knowledge of the *in situ* physical and chemical state of the contaminant. A first-order problem in characterizing the *in situ* state of non-aqueous phase contaminants is determining the pore-scale distribution and mobility of the contaminant. Of specific interest in this research is determining the wettability of the system; i.e. is the contaminant present as an immiscible *non-wetting* phase located in the central volume of the pore space, or does the contaminant exist as a *wetting* phase that is adsorbed to, or coating, the solid surface. We plan to investigate, through an extensive laboratory study, the concept that measurements of the dielectric constant and nuclear magnetic resonance (NMR) can be used to determine wettability and thus discriminate between these two cases.

Wettability is defined as the tendency of one fluid to adsorb to, or to coat, a solid surface in the presence of other immiscible fluids (Craig, 1971). Water strongly wets most rock-forming minerals, but some oils, for example, can "out-compete" the water for the solid surface causing the "water-wet" rock to become "oil-wet". The wettability is a critical factor in determining the pore-scale location of the immiscible fluids and the movement of the fluid phases. While studies of wettability have long been an important part of understanding and modeling multi-phase flow in hydrocarbon reservoirs, there has been relatively little attention paid to the role of wettability in contaminant transport and remediation, even when the contaminant is an oil. In fact, it is generally assumed in an oil-water-air system that water is the wetting phase. As reviewed in a recent paper (Bradford and Leiji, 1996) this is not true for many natural systems, and the assumption of a water-wet state can lead to grossly inaccurate predictions of capillary pressure-saturation relationships, and the mobility of the contaminant. Determining wettability is thus a critical factor in site characterization.

Our past research has clearly shown a link between the dielectric and NMR response of geological materials and the wettability of the material. This has introduced the intriguing possibility that the combined use of dielectric and NMR measurements can be used as a means of characterizing the wettability of a geological system. For field applications, ground penetrating radar (GPR) is a high frequency electromagnetic technique that can be used to measure the dielectric properties of the subsurface in the frequency range of 10 MHz to 1 GHz. The current development of a geophysical technique referred to as very early time electromagnetics (VETEM) will provide a means of obtaining measurements of dielectric properties at lower frequencies, in the range of 10 kHz to 150 MHz (Pellerin et al., 1995). Measurement of the *in situ* NMR response of materials in the subsurface can be made with NMR borehole systems, and by using a surface measurement system, recently developed and now commercially available. The interest in this research is the potential use of both GPR and/or VETEM, and NMR as a means of characterizing the *in situ* physical and chemical state of an organic contaminant in the subsurface.

The objectives of the research do not involve any analysis of the field methods. The use of the field techniques provides information about the dielectric constant and the NMR relaxation time of the subsurface. Our focus is exclusively a laboratory study aimed at developing a fundamental understanding of the link these two parameters and the pore-scale location of a conaminationt. Specifically - can we discriminate, with dielectric and NMR measurements, between a water-wet system in which water coats the solid surface, and a system in which an organic contaminant is absorbed to the solid?

We will first prepare a suite of unconsolidated samples with varying wettability; then measure both the dielectric and NMR response of the samples as a function of solution chemistry. Both the composition of the wetting film and solution chemistry can affect wettability and will be the two key parameters in this study. The results of this comprehensive laboratory study will provide us with the data set necessary to both model and predict the dependence of dielectric properties and NMR on wettability. This will contribute significantly to a long-term research objective which is to assess the combined use of GPR and/or VETEM, and NMR to discriminate, *in situ,* between the wetting versus non-wetting behavior of contaminants.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

Environmental Management Science Program Research in Ontario, Canada

University of Toronto

54790-CAN-ON - Microbial Mineral Transformations at the Fe(II)/Fe(III) Redox Boundary for Solid Phase Capture of Strontium and Other Metal/Radionuclide Contaminants

Year of Award: 1996 **Amount of Award:** $502,393
Problem Area: Remedial Action
Science Category/SubCategory: Biogeochemistry / Biogeochemistry
Principal Investigator: Dr. F. Grant Ferris, 416-978-3022, ferris@quartz.geology.utoronto.ca
Major Collaborator(s): Eric Roden at the University of Alabama
For More Information: http://www.doe.gov/em52/54790.html

Description Provided by Investigator:

Studies at The University of Alabama and the University of Toronto will determine microbiological and geochemical controls on carbonate mineral precipitation reactions that are caused by bacterial reduction of Fe(III) oxides, and identify contributions of there processes to the solid phase capture of strontium and other metal/radionuclide contaminants. The impact of microbial Fe(III) oxide reduction on Sr chemistry will be addressed in sequential manner, starting with batch aqueous suspension experiments. These will be followed by microcosm semicontinuous culture studies using saturated sands artificially coated with Fe(III) oxides and natural Fe(III) oxide bearing sediments. Constant hydraulic head flow-through column experiments will ultimately be conducted to assess aqueous and solid phase distribution of strontium under simulated field conditions.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Remedial Action problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Remedial Action".

The following projects were identified through systems engineering as potentially having needs that can be addressed through this research award. Those projects that may have the strongest link to this award are designated by the symbol "§".

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
§+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
§+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
§ RL-ER08	C-147	Groundwater Management
§+ SR-ER06	C-227	Upper Three Runs Project

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High Level Waste

Projects in the High Level Waste Environmental Management Problem Area.

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
ID-HLW-101	C-29	High-Level Waste Pretreatment
ID-HLW-102	C-33	High-Level Waste Immobilization Facility (Privatized)
+ ID-HLW-103	C-35	High-Level Waste Treatment and Storage
+ RL-TW04	C-169	Retrieval Project
+ RL-TW05	C-173	Process Waste Support
+ RL-TW06	C-177	Process Waste Privatization Phase I
+ RL-TW07	C-181	Process Waste Privatization Phase II
+ RL-TW08	C-185	Process Waste Privatization Infrastructure
RL-TW09	C-187	Immobilized Tank Waste Storage & Disposal Project
+ RL-WM05	C-201	Liquid Effluents Project
+ SR-HL01	C-249	H-Tank Farm
+ SR-HL02	C-253	F-Tank Farm
SR-HL03	C-257	Waste Removal Operations and Tank Closure
+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
SR-HL05	C-265	Vitrification
SR-HL08	C-269	Saltstone
SR-HL12	C-271	High Level Waste System Upgrades

Spent Nuclear Fuel

Projects in the Spent Nuclear Fuel Environmental Management Problem Area.

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
ID-SNF-102	C-39	Integrated Spent Nuclear Fuel Program
RL-WM02	C-191	Canister Storage Building Operations
+ SR-SF02	C-275	L-Reactor Spent Nuclear Fuel Project
SR-SF03	C-277	Recceving Basin for Off-site Fuels (RBOF) Spent Nuclear Fuel Project
+ SR-SF09	C-279	Spent Nuclear Fuel Transfer and Storage

Index of High Cost Environmental Management Projects by Problem Area Continued

Mixed Waste

Projects in the Mixed Waste Environmental Management Problem Area.

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
ID-WM-105	C-41	Advanced Mixed Waste Treatment Project (AMWTP) Production Operations
ID-WM-107	C-45	Long Term Treatment/Storage/Disposal Operations
+ OR-38111	C-61	Mixed Low Level Waste Management
RL-ER04	C-137	Environmental Restoration Disposal Facility
RL-WM03	C-193	Solid Waste Storage and Disposal
RL-WM04	C-197	Solid Waste Treatment
+ RL-ST01	C-205	PNNL WASTE MANAGEMENT
RF002	C-209	Waste Management Project
+ SR-SW01	C-281	Consolidated Incinerator Facility
+ SR-SW02	C-285	Transuranic Waste Project
+ SR-SW03	C-287	Mixed Low Level Waste Project
+ SR-SW04	C-291	Low Level Waste Project

Nuclear Materials

Projects in the Nuclear Materials Environmental Management Problem Area.

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
+ RL-TP02	C-153	Waste Encapsulation and Storage Facility (WESF) Sub-Project
+ RL-TP07	C-161	Plutonium Finishing Plant (PFP) Vault Management
SR-NM06	C-273	Nuclear Materials Storage

Remedial Action

Projects in the Remedial Action Environmental Management Problem Area.

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
AL024	C-3	Grand Junction Office (GJO) All Other Projects
AL007	C-7	Environmental Restoration
AL009	C-9	LANL Environmental Restoration
+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
ID-ER-106	C-23	Radioactive Waste Management Complex Remediation
ID-ER-109	C-25	Remediation Operations
NV212	C-49	Underground Test Area (UGTA)
NV214	C-53	Industrial Sites
OR-42101	C-63	Y-12 East Fork Poplar Creek Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
+ OR-48101	C-99	Offsite Remedial Action
+ OR-45301	C-103	Paducah Remedial Action

Index of High Cost Environmental Management Projects by Problem Area Continued

Remedial Action Continued

Project ID	Page #	Project Title
+ OR-46301	C-107	Portsmouth Remedial Action
+ OH-FN-07	C-115	Silos
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
RL-ER08	C-147	Groundwater Management
RF013	C-211	Closure Caps Project
RF014	C-213	Industrial Zone Closure Project
SR-ER03	C-223	Lower Three Runs & Operations Project
+ SR-ER06	C-227	Upper Three Runs Project

Decontamination and Decommissioning

Projects in the Decontamination and Decommissioning Environmental Management Problem Area.

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
+ AL013	C-11	LANL Waste Management - Legacy Waste
ID-ER-110	C-27	Decontamination and Decommissioning
ID-OIM-113	C-37	Post-2006 Surveillance, Maintenance, and Monitoring
+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
OR-43204	C-77	ORNL Bethel Valley Deactivation and Decommissioning
OR-44302	C-87	East Tennessee Technology Park (ETTP) Process Equipment D&D
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
SP-SPRU	C-111	Separations Process Research Unit (SPRU)
+ RL-ER05	C-139	Facility Surveillance & Maintenance - ADS 3500
+ RL-ER06	C-141	Decontamination and Decommissioning
RL-ER07	C-145	Post Closure Surveillance & Maintenance
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
RL-TP10	C-163	Accelerated Deactivation
+ RL-TP13	C-167	Landlord Project
SR-FA02	C-233	F Canyon Deactivation Project
SR-FA04	C-235	H Canyon Deactivation Project
SR-FA06	C-237	235-F Deactivation Project
SR-FA16	C-239	F-Area Monitoring
SR-FA17	C-241	H-Area Monitoring and Minor Facility Monitoring
SR-FA18	C-243	M Area Monitoring Project
SR-FA20	C-245	Reactors Monitoring Project
SR-FA22	C-247	Receiving Basin for Off-site Fuels (RBOF) Monitoring Project

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Health / Ecology / Risk

Projects in the Health / Ecology / Risk Environmental Management Problem Area.

"+" Designates projects which must remain active in the year 2007 and beyond to manage high risks.

Project ID	Page #	Project Title
+ AL013	C-11	LANL Waste Management - Legacy Waste
+ ID-ER-103	C-17	Idaho Chemical Processing Plant Remediation
+ ID-HLW-103	C-35	High-Level Waste Treatment and Storage
+ OR-38111	C-61	Mixed Low Level Waste Management
+ OR-43202	C-69	ORNL Melton Valley Watershed Remedial Action
+ OR-43203	C-73	ORNL Bethel Valley Remedial Action
+ OR-44301	C-81	East Tennessee Technology Park (ETTP) Remedial Action
+ OR-44303	C-93	East Tennessee Technology Park (ETTP) D&D
+ OR-48101	C-99	Offsite Remedial Action
+ OR-45301	C-103	Paducah Remedial Action
+ OR-46301	C-107	Portsmouth Remedial Action
+ OH-FN-07	C-115	Silos
+ RL-ER01	C-125	100 Area Remedial Action
+ RL-ER02	C-129	200 Area Remedial Action
+ RL-ER03	C-133	300 Area Remedial Action
+ RL-ER05	C-139	Facility Surveillance & Maintenance - ADS 3500
+ RL-ER06	C-141	Decontamination and Decommissioning
+ RL-TP02	C-153	Waste Encapsulation and Storage Facility (WESF) Sub-Project
+ RL-TP05	C-155	Plutonium Finishing Plant Deactivation
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+ SR-HL04	C-261	In Tank Precipitation/Extended Sludge Processing/Late Wash (ITP/ESP/LW) Operations
+ SR-SF02	C-275	L-Reactor Spent Nuclear Fuel Project
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55137-CA	B-53	Investigation of Novel Electrode Materials for Electrochemically-Based Remediation of High- and Low-Level Mixed Wastes in the DOE Complex
54656-CA	B-65	Mixing Processes in High-Level Waste Tanks
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55042-GA	B-105	Quantifying Silica Reactivity in Subsurface Environments: Controls of Reaction Affinity and Solute Matrix on Quartz and SiO2 Glass Dissolution Kinetics
60424-ID	B-113	High Temperature Condensed Phase Mass Spectrometric Analysis
55229-IL	B-117	The NOx System in Nuclear Waste
55294-IL	B-121	Superconducting Open-Gradient Magnetic Separation for the Pretreatment of Radioactive or Mixed Waste Vitrification Feeds
55367-IL	B-123	Investigation of Microscopic Radiation Damage in Waste Forms Using ODNMR and AEM Techniques
60313-IL	B-135	Radiation Effects on Transport and Bubble Formation in Silicate Glasses
60143-IL	B-137	Foaming in Radioactive Waste Treatment and Immobilization Processes
59977-MD	B-169	Synthesis and Characterization of Templated Ion Exchange Resins for the Selective Complexation of Actinide Ions
55141-MA	B-177	Imaging and Characterizing the Waste Materials Inside an Underground Storage Tank Using Seismic Normal Modes
54691-MI	B-189	Radiation Effects on Materials in the Near-Field of Nuclear Waste Repository
54765-NM	B-211	Enhanced Sludge Processing of HLW: Hydrothermal Oxidation of Chromium, Technetium, and Complexants by Nitrate
54773-NM	B-215	Microstructural Properties of High Level Waste Concentrates and Gels with Raman And Infrared Spectroscopies
59990-NM	B-221	Fundamental Chemistry, Characterization, and Separation of Technetium Complexes in Hanford Waste
59993-NM	B-223	Dynamic Effects of Tank Waste Aging on Radionuclide-Complexant Interactions
60403-NM	B-243	Phase Chemistry of Tank Sludge Residual Components
54595-NM	B-255	f-Element Ion Chelation in Highly Basic Media
59982-NY	B-259	Reactivity of Peroxynitrite: Implications for Hanford Waste Management and Remediation
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54674-OH	B-271	Design and Development of a New Hybrid Spectroelectrochemical Sensor
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55087-TN	B-309	Design and Synthesis of the Next Generation of Crown Ethers for Waste Separations: An Inter-Laboratory Comprehensive Proposal
59978-TN	B-321	Thermospray Mass Spectrometry Ionization Processes Fundamental Mechanisms for Speciation, Separation and Characterization of Organic Complexants in DOE Wastes
60020-TN	B-323	Stability of High-Level Waste Forms
60217-TN	B-331	Optically-Based Array Sensors for Selective In Situ Analysis of Tank Waste
54735-TX	B-343	Development of Inorganic Ion Exchangers for Nuclear Waste Remediation
54621-WA	B-357	Chemical Speciation of Strontium, Americium, and Curium in High Level Waste: Predictive Modeling of Phase Partitioning During Tank Processing
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60345-WA	B-375	New Silicotitanate Waste Forms: Development and Characterization
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54847-CO	B-87	Photocatalytic and Chemical Oxidation of Organic Compounds in Supercritical Carbon Dioxide
55012-CO	B-89	Extraction and Recovery of Mercury and Lead from Aqueous Waste Streams Using Redox-active Layered Metal Chalcogenides
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55110-MO	B-195	An Alternative Host Matrix Based on Iron Phosphate Glasses for the Vitrification of Specialized Nuclear Waste Forms
55223-MO	B-197	De Novo Design of Ligands for Metal Separation
54751-NM	B-209	High Fluence Neutron Source for Nondestructive Characterization of Nuclear Waste
54770-NM	B-213	New Anion-Exchange Resins for Improved Separations of Nuclear Materials
59981-NM	B-219	Real-Time Broad Spectrum Characterization of Hazardous Waste by Membrane Introduction Mass Spectrometry
55387-NM	B-237	Photooxidation of Organic Wastes Using Semiconductor Nanoclusters
55171-PA	B-283	Development of Advanced In-Situ Techniques for Chemistry Monitoring and Corrosion Mitigation in SCWO Environments
54828-SC	B-297	Processing of High Level Waste: Spectroscopic Characterization of Redox Reactions in Supercritical Water
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54897-WA	B-391	The Sonophysics and Sonochemistry of Liquid Waste Quantification and Remediation
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55382-IL	B-129	Determination of Transmutation Effects in Crystalline Waste Forms
60247-IL	B-139	Miniature Nuclear Magnetic Resonance Spectrometer for In-Situ and In-Process Analysis and Monitoring
59967-NM	B-217	Aqueous Electrochemical Mechanisms in Actinide Residue Processing
60118-NM	B-229	Fundamental Thermodynamics of Actinide-Bearing Mineral Waste Forms
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54908-AZ	B-7	Partitioning Tracers for In Situ Detection and Quantification of Dense Nonaqueous Phase Liquids in Groundwater Systems
55097-CA	B-15	Heavy Metal Pumps in Plants
55278-CA	B-17	Molecular Genetics of Metal Detoxification: Prospects for Phytoremediation
54698-CA	B-19	Rapid Mass Spectrometric DNA Diagnostics for Assessing Microbial Community Activity During Bioremediation
55264-CA	B-21	Subsurface High Resolution Definition of Subsurface Heterogeneity for Understanding the Biodynamics of Natural Field Systems: Advancing the Ability for Scaling to Field Conditions
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55011-CA	B-43	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes
55148-CA	B-45	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry Measurements
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55041-CA	B-79	Molecular Characterization of a Novel Heavy Metal Uptake Transporter from Higher Plants & its Potential for Use in Phytoremediation
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55105-MI	B-183	Complete Detoxification of Short Chain Chlorinated Aliphatics: Isolation of Halorespiring Organisms and Biochemical Studies of the Dehalogenating Enzyme Systems
54548-MI	B-185	The Efficacy of Oxidative Coupling for Promoting In-Situ Immobilization of Hydroxylated Aromatics in Contaminated Soil and Sediment Systems
54680-MI	B-187	The Migration and Entrapment of DNAPLs in Physically and Chemically Heterogeneous Porous Media
60271-NH	B-199	Characterization of a New Family of Metal Transport Proteins
54741-NM	B-207	Characterization of Contaminant Transport Using Naturally-Occurring U-Series Disequilibria
59996-NM	B-225	Plutonium Speciation, Solubilization, and Migration in Soils
55332-NM	B-235	A Hybrid Hydrologic-Geophysical Inverse Technique for the Assessment and Monitoring of Leachates in the Vadose Zone
55395-NM	B-239	Physics of DNAPL Migration and Remediation in the Presence of Heterogeneities
54857-NM	B-245	Surface Nuclear Magnetic Resonance Imaging of Water Content Distribution in the Subsurface
55109-NM	B-247	New Permeameters for in situ Characterization of Unsaturated Heterogeneous Permeability
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54823-NM	B-253	Modeling of Cation Binding in Hydrated 2:1 Clay Minerals
54793-NY	B-263	Establishing a Quantitative Functional Relationship Between Capillary Pressure Saturation and Interfacial Area
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55196-OR	B-277	In Situ, Field Scale Evaluation of Surfactant Enhanced DNAPL Recovery Using a Single-Well, Push-Pull Test
60158-OR	B-279	Development of Radon-222 as a Natural Tracer for Monitoring the Remediation of NAPL Contamination in the Subsurface
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55205-SC	B-299	A Fundamental Study of Laser-Induced Breakdown Spectroscopy Using Fiber Optics for Remote Measurements of Trace Metals
55013-TN	B-303	Biofiltration of Volatile Pollutants: Engineering Mechanisms for Improved Design, Long-term Operation, Prediction and Implementation
55033-TN	B-305	Characterization of Chemically Modified Hyperthermophilic Enzymes for Chemical Syntheses and Bioremediation Reactions
55036-TN	B-307	Colloid Transport and Retention in Fractured Deposits
55108-TN	B-313	Monitoring Genetic & Metabolic Potential for In Situ Bioremediation: Mass Spectrometry
55119-TN	B-315	Phase Equilibria Modification by Electric Fields
55267-TN	B-317	Containment of Toxic Metals and Radionuclides in Porous and Fractured Media: Optimizing Biogeochemical Reduction versus Geochemical Oxidation
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55185-TX	B-349	New Strategies for Designing Inexpensive but Selective Bioadsorbants for Environmental Pollutants: Selection of Specific Ligands & Their Cell Surface Expression
55216-TX	B-351	In-Situ Characterization of Dense Non-Aqueous Phase Liquids Using Partitioning Tracers
60069-VT	B-355	Least-Cost Groundwater Remediation Design Using Uncertain Hydrogeological Information
54635-WA	B-361	Molecular-Level Process Governing the Interaction of Contaminants with Iron and Manganese Oxides
55031-WA	B-373	Genetic Analysis of Stress Responses in Soil Bacteria for Enhanced Bioremediation of Mixed Contaminants
60355-WA	B-377	Mineral Surface Processes Responsible for the Decreased Retardation (or Enhanced Mobilization) of 137Cs from HLW Tank Discharges
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54889-WA	B-389	Using Trees to Remediate Groundwaters Contaminated with Chlorinated Hydrocarbons
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54790-CAN-ON	B-407	Microbial Mineral Transformations at the Fe(II)/Fe(III) Redox Boundary for Solid Phase Capture of Strontium and Other Metal/Radionuclide Contaminants

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60283-IL	B-133	Waste Volume Reduction Using Surface Characterization and Decontamination by Laser Ablation
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60363-NM	B-241	Optimization of Thermochemical, Kinetic, and Electrochemical Factors Governing Partitioning of Radionuclides during Melt Decontamination of Radioactively Contaminated Stainless Steel
60040-NY	B-257	Development of Monitoring and Diagnostic Methods for Robots Used in Remediation of Waste Sites
60041-OK	B-275	Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration
55052-SC	B-295	Advanced Sensing and Control Techniques to Facilitate Semi-Autonomous Decommissioning
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60163-NM	B-249	Investigation of Techniques to Improve Continuous Air Monitors Under Conditions of High Dust Loading in Environmental Setting
55100-NY	B-261	Human Genetic Marker for Resistance to Radiations and Chemicals
59882-NY	B-265	Measurements of Radon, Thoron, Isotopic Uranium and Thorium to Determine Occupational & Environmental Exposure & Risk at Fernald Feed Materials Production Center
60474-OH	B-273	Develop and Demonstrate Novel Ultrahigh Sensitivity Heavy Noble Gas Detectors for Long-Term Monitoring of Spent Fuel and TRU Waste
54856-PA	B-289	Structural Biology of the Sequestration & Transport of Heavy Metal Toxins: NMR Structure Determination of Proteins Containing the -Cys-X-Y-Cys-metal Binding Motifs
55410-SC	B-291	Determining Significant Endpoints for Ecological Risk Analyses
60037-TN	B-325	Estimation of Potential Population Level Effects of Contaminants on Wildlife
60218-TN	B-333	Novel Mass Spectrometry Mutation Screening for Contaminant Impact Analysis
54931-VT	B-353	A Novel Biomarker for Beryllium Sensitization in Humans
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Actinide (Heavy Element) Chemistry

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54893-FL	B-99	Research Program to Determine Redox Properties and Their Effects on Speciation and Mobility of Pu in DOE Wastes
59977-MD	B-169	Synthesis and Characterization of Templated Ion Exchange Resins for the Selective Complexation of Actinide Ions
54683-MA	B-173	Speciation and Structural Characterization of Plutonium and Actinide-organic Complexes in Surface and Groundwaters
59967-NM	B-217	Aqueous Electrochemical Mechanisms in Actinide Residue Processing
59996-NM	B-225	Plutonium Speciation, Solubilization, and Migration in Soils
54595-NM	B-255	f-Element Ion Chelation in Highly Basic Media
54621-WA	B-357	Chemical Speciation of Strontium, Americium, and Curium in High Level Waste: Predictive Modeling of Phase Partitioning During Tank Processing
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60075-WA	B-401	Particle Generation by Laser Ablation in Support of Chemical Analysis of High Level Mixed Waste from Plutonium Production Operations

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54864-KS	B-157	Supramolecular Chemistry of Selective Anion Recognition for Anions of Environmental Relevance
60231-MD	B-165	Novel Miniature Spectrometer for Remote Chemical Detection
60070-MS	B-193	The Development of Cavity Ringdown Spectroscopy as a Sensitive Continuous Emission Monitor for Metals
54751-NM	B-209	High Fluence Neutron Source for Nondestructive Characterization of Nuclear Waste
60163-NM	B-249	Investigation of Techniques to Improve Continuous Air Monitors Under Conditions of High Dust Loading in Environmental Setting
54639-NM	B-251	Development of an In-Situ Microsensor for the Measurements of Chromium and Uranium in Groundwater at DOE Sites
54674-OH	B-271	Design and Development of a New Hybrid Spectroelectrochemical Sensor
60474-OH	B-273	Develop and Demonstrate Novel Ultrahigh Sensitivity Heavy Noble Gas Detectors for Long-Term Monitoring of Spent Fuel and TRU Waste
55171-PA	B-283	Development of Advanced In-Situ Techniques for Chemistry Monitoring and Corrosion Mitigation in SCWO Environments
60219-PA	B-287	Development of Advanced Electrochemical Emission Spectroscopy for Monitoring Corrosion in Simulated DOE Liquid Waste
60197-TN	B-329	Microsensors for In-situ Chemical, Physical, and Radiological Characterization of Mixed Waste
60217-TN	B-331	Optically-Based Array Sensors for Selective In Situ Analysis of Tank Waste
55328-TN	B-337	Novel Analytical Techniques Based on an Enhanced Electron Attachment Process
54800-WA	B-387	Construction of Bending Magnet Beamline at the APS for Environmental Studies
55146-WA	B-393	Adsorption/Membrane Filtration as a Contaminant Concentration and Separation Process for Mixed Wastes and Tank Wastes

Biogeochemistry

Biogeochemistry

Award ID	Page #	Award Title
55164-AL	B-3	Advanced Experimental Analysis of Controls on Microbial Fe(III) Oxide Reduction
55388-IL	B-131	Stable Isotopic Investigations of in situ Bioremediation of Chlorinated Organic Solvents
55071-ME	B-163	Reduction and Immobilization of Radionuclides and Toxic Metal Ions Using Combined Zero Valent Iron and Anaerobic Bacteria
60015-NM	B-227	Long-term Risk from Actinides in the Environment: Modes of Mobility
55267-TN	B-317	Containment of Toxic Metals and Radionuclides in Porous and Fractured Media: Optimizing Biogeochemical Reduction versus Geochemical Oxidation
54790-CAN-ON	B-407	Microbial Mineral Transformations at the Fe(II)/Fe(III) Redox Boundary for Solid Phase Capture of Strontium and Other Metal/Radionuclide Contaminants

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Engineering Science

Bioengineering

Award ID	Page #	Award Title
55013-TN	B-303	Biofiltration of Volatile Pollutants: Engineering Mechanisms for Improved Design, Long-term Operation, Prediction and Implementation

Bubble Mechanics and Sonification

Award ID	Page #	Award Title
55374-IL	B-125	Use of Sonication for In-Well Softening of Semivolatile Organic Compounds
60143-IL	B-137	Foaming in Radioactive Waste Treatment and Immobilization Processes
55211-IL	B-141	Cavitational Hydrothermal Oxidation: A New Remediation Process
54973-TN	B-301	A Novel Energy-Efficient Plasma Chemical Process for the Destruction of Volatile Toxic Compounds
60451-WA	B-385	Mechanics of Bubbles in Sludges and Slurries

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Award ID	Page #	Award Title
60326-AZ	B-11	Isolation of Metals from Liquid Wastes: Reactive Scavenging in Turbulent Thermal Reactors
54656-CA	B-65	Mixing Processes in High-Level Waste Tanks
60155-CO	B-83	Measurements and Models for Hazardous Chemical and Mixed Wastes
60144-ID	B-115	Flow Visualization of Forced and Natural Convection in Internal Cavities
60077-TN	B-327	Development of Nuclear Analysis Capabilities for DOE Waste Management Activities

Diagnostics

Award ID	Page #	Award Title
54890-CA	B-69	On-Line Slurry Viscosity and Concentration Measurement as a Real-Time Waste Stream Characterization Tool
55294-IL	B-121	Superconducting Open-Gradient Magnetic Separation for the Pretreatment of Radioactive or Mixed Waste Vitrification Feeds
54857-NM	B-245	Surface Nuclear Magnetic Resonance Imaging of Water Content Distribution in the Subsurface
55179-NY	B-267	Acoustic Probe for Solid-Gas-Liquid Suspensions

Robotics

Award ID	Page #	Award Title
60040-NY	B-257	Development of Monitoring and Diagnostic Methods for Robots Used in Remediation of Waste Sites
55052-SC	B-295	Advanced Sensing and Control Techniques to Facilitate Semi-Autonomous Decommissioning

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Geochemistry

Colloidal Chemistry and Transport

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55284-CA	B-55	Aquifer Transport of Th, U, Ra, and Rn in Solution and on Colloids

Solid/Solution Geochemistry

Award ID	Page #	Award Title
59960-IN	B-151	Direct Investigations of the Immobilization of Radionuclides in the Alteration Phases of Spent Nuclear Fuel
59849-MI	B-191	Radionuclide Immobilization in the Phases Formed by Corrosion of Spent Nuclear Fuel: The Long-Term Assessment

Sorption/Desorption

Award ID	Page #	Award Title
55014-AL	B-1	Kinetics and Mechanisms of Metal Retention/Release in Geochemical Processes in Soil
55396-CA	B-33	Sorption of Colloids, Organics, and Metals onto Gas-Water Interfaces: Transport Mechanisms and Potential Remediation Technology
55148-CA	B-45	Hydrologic and Geochemical Controls on the Transport of Radionuclides in Natural Undisturbed Arid Environments as Determined by Accelerator Mass Spectrometry Measurements
55249-CA	B-47	Experimental Determination of Contaminant Metal Mobility as a Function of Temperature Time and Solution Chemistry
54860-CA	B-59	Sorption of Heavy Metals and Radionuclides on Mineral Surfaces in the Presence of Organic Co-Contaminants
55042-GA	B-105	Quantifying Silica Reactivity in Subsurface Environments: Controls of Reaction Affinity and Solute Matrix on Quartz and SiO2 Glass Dissolution Kinetics
54548-MI	B-185	The Efficacy of Oxidative Coupling for Promoting In-Situ Immobilization of Hydroxylated Aromatics in Contaminated Soil and Sediment Systems
54741-NM	B-207	Characterization of Contaminant Transport Using Naturally-Occurring U-Series Disequilibria
60403-NM	B-243	Phase Chemistry of Tank Sludge Residual Components
54823-NM	B-253	Modeling of Cation Binding in Hydrated 2:1 Clay Minerals
54585-OH	B-269	Permanganate Treatment of DNAPLs in Reactive Barriers and Source Zone Flooding Schemes
54635-WA	B-361	Molecular-Level Process Governing the Interaction of Contaminants with Iron and Manganese Oxides
60355-WA	B-377	Mineral Surface Processes Responsible for the Decreased Retardation (or Enhanced Mobilization) of 137Cs from HLW Tank Discharges

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55011-CA	B-43	Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes
55411-CA	B-49	Joint Inversion of Geophysical Data for Site Characterization and Restoration Monitoring
54655-CA	B-63	Collaborative Research: Hydrogeological-Geophysical Methods for Subsurface Site Characterization
60162-CO	B-85	Enhancements to and Characterization of the Very Early Time Electromagnetic (VETEM) Prototype Instrument and Applications to Shallow Subsurface Imaging at Sites in the DOE Complex
55218-GA	B-107	Seismic Surface-Wave Tomography of Waste Sites
60199-KS	B-159	Seismic-Reflection and Ground Penetrating Radar for Environmental Site Characterization
55141-MA	B-177	Imaging and Characterizing the Waste Materials Inside an Underground Storage Tank Using Seismic Normal Modes
55300-MA	B-179	3-D Spectral IP Imaging: Non-Invasive Characterization of Contaminant Plumes
55332-NM	B-235	A Hybrid Hydrologic-Geophysical Inverse Technique for the Assessment and Monitoring of Leachates in the Vadose Zone
60115-TX	B-341	Advanced High Resolution Seismic Imaging, Material Properties Estimation and Full Wavefield Inversion for the Shallow Subsurface
54699-CAN-BC	B-405	The Use of Dielectric and NMR Measurements to Determine the Pore-Scale Location of Organic Contaminants

Health Science

Biophysics/Dose

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54584-NJ	B-201	Comparison of the Bioavailability of Elemental Waste Laden Soils Using in vivo and in vitro Analytical Methodology, and Refinement of Exposure/Dose Models
59918-NM	B-233	Improved Radiation Dosimetry/Risk Estimates to Facilitate Environmental Management of Plutonium Contaminated Sites
59882-NY	B-265	Measurements of Radon, Thoron, Isotopic Uranium and Thorium to Determine Occupational & Environmental Exposure & Risk at Fernald Feed Materials Production Center

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Award ID	Page #	Award Title
55356-CA	B-29	Environmentally-induced Malignancies: An In Vivo Model to Evaluate the Health Impact of Chemicals in Mixed Waste
55032-LA	B-161	Environmental Analysis of Endocrine Disrupting Effects from Hydrocarbon Contaminants in the Ecosystem
54684-WA	B-369	Mechanism Involved in Trichloroethylene-Induced Liver Cancer: Importance to Environmental Cleanup

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54546-CA	B-61	Engineered Antibodies for Monitoring of Polynuclear Aromatic Hydrocarbons
55100-NY	B-261	Human Genetic Marker for Resistance to Radiations and Chemicals
54856-PA	B-289	Structural Biology of the Sequestration & Transport of Heavy Metal Toxins: NMR Structure Determination of Proteins Containing the -Cys-X-Y-Cys-metal Binding Motifs
55033-TN	B-305	Characterization of Chemically Modified Hyperthermophilic Enzymes for Chemical Syntheses and Bioremediation Reactions
55185-TX	B-349	New Strategies for Designing Inexpensive but Selective Bioadsorbants for Environmental Pollutants: Selection of Specific Ligands & Their Cell Surface Expression
54931-VT	B-353	A Novel Biomarker for Beryllium Sensitization in Humans

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59828-CA	B-81	Bioavailability of Organic Solvents in Soils: Input into Biologically Based Dose-Response Models for Human Risk Assessments
54940-NM	B-231	Improved Risk Estimates for Carbon Tetrachloride
55410-SC	B-291	Determining Significant Endpoints for Ecological Risk Analyses
60037-TN	B-325	Estimation of Potential Population Level Effects of Contaminants on Wildlife

Hydrogeology

Dense Non-Aqueous Phase Liquid (DNAPL) Dynamics

Award ID	Page #	Award Title
54908-AZ	B-7	Partitioning Tracers for In Situ Detection and Quantification of Dense Nonaqueous Phase Liquids in Groundwater Systems
54680-MI	B-187	The Migration and Entrapment of DNAPLs in Physically and Chemically Heterogeneous Porous Media
55395-NM	B-239	Physics of DNAPL Migration and Remediation in the Presence of Heterogeneities
55196-OR	B-277	In Situ, Field Scale Evaluation of Surfactant Enhanced DNAPL Recovery Using a Single-Well, Push-Pull Test
60158-OR	B-279	Development of Radon-222 as a Natural Tracer for Monitoring the Remediation of NAPL Contamination in the Subsurface
55083-TN	B-335	Behavior of Dense, Immiscible Solvents in Fractured Clay-Rich Soils
55216-TX	B-351	In-Situ Characterization of Dense Non-Aqueous Phase Liquids Using Partitioning Tracers

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54888-MA	B-175	Manipulating Subsurface Colloids to Enhance Cleanups of DOE Waste Sites
55036-TN	B-307	Colloid Transport and Retention in Fractured Deposits

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54950-CA	B-41	Characterization of Contaminant Transport by Gravity, Capillarity and Barometric Pumping in Heterogeneous Vadose Regimes
54576-IN	B-145	On the Inclusion of the Interfacial Area Between Phases in the Physical and Mathematical Description of Subsurface Multiphase Flow
55109-NM	B-247	New Permeameters for in situ Characterization of Unsaturated Heterogeneous Permeability
54793-NY	B-263	Establishing a Quantitative Functional Relationship Between Capillary Pressure Saturation and Interfacial Area
60069-VT	B-355	Least-Cost Groundwater Remediation Design Using Uncertain Hydrogeological Information

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Hydrothermal Oxidation

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54765-NM	B-211	Enhanced Sludge Processing of HLW: Hydrothermal Oxidation of Chromium, Technetium, and Complexants by Nitrate
54828-SC	B-297	Processing of High Level Waste: Spectroscopic Characterization of Redox Reactions in Supercritical Water
55276-TN	B-319	Fundamental Chemistry and Thermodynamics of Hydrothermal Oxidation Processes
54506-TX	B-347	Acid-Base Behavior in Hydrothermal Processing of Wastes

Multiphase/Gaseous Chemistry

Award ID	Page #	Award Title
55137-CA	B-53	Investigation of Novel Electrode Materials for Electrochemically-Based Remediation of High- and Low-Level Mixed Wastes in the DOE Complex
54807-GA	B-103	Studies Related to Chemical Mechanisms of Gas Formation in Hanford High-Level Nuclear Wastes
54834-IN	B-143	An Investigation of Homogeneous and Heterogeneous Sonochemistry for Destruction of Hazardous Waste
59934-IN	B-149	Hazardous Gas Production by Alpha Particles in Solid Organic Transuranic Waste Matrices
55119-TN	B-315	Phase Equilibria Modification by Electric Fields
54897-WA	B-391	The Sonophysics and Sonochemistry of Liquid Waste Quantification and Remediation

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60296-CA	B-35	Research Program to Investigate the Fundamental Chemistry of Technetium
55061-CA	B-77	Fundamental Studies of the Removal of Contaminants from Ground and Waste Waters via Reduction by Zero-Valent Metals
55229-IL	B-117	The NOx System in Nuclear Waste
54724-NM	B-205	Synthesis of New Water-Soluble Metal-Binding Polymers: Combinatorial Chemistry Approach
55115-TX	B-345	The Adsorption and Reaction of Halogenated Volatile Organic Compounds (VOC's) on Metal Oxides
54628-WA	B-359	Colloidal Agglomerates in Tank Sludge: Impact on Waste Processing
54646-WA	B-363	Interfacial Radiolysis Effects in Tank Waste Speciation

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Chemical and Structural Properties Of Storage Materials

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55094-CA	B-13	Chemical and Ceramic Methods Toward Safe Storage of Actinides Using Monazite
54982-FL	B-101	Analysis of Surface Leaching Processes in Vitrified High-Level Nuclear Wastes Using In-Situ Raman Imaging and Atomistic Modeling
55110-MO	B-195	An Alternative Host Matrix Based on Iron Phosphate Glasses for the Vitrification of Specialized Nuclear Waste Forms
60118-NM	B-229	Fundamental Thermodynamics of Actinide-Bearing Mineral Waste Forms
60020-TN	B-323	Stability of High-Level Waste Forms
60345-WA	B-375	New Silicotitanate Waste Forms: Development and Characterization
60362-WA	B-379	Ion-Exchange Processes and Mechanisms in Glasses
60387-WA	B-381	Distribution & Solubility of Radionuclides & Neutron Absorbers in Waste Forms for Disposition of Plutonium Ash & Scraps, Excess Plutonium, and Miscellaneous Spent Nuclear Fuels

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59827-AZ	B-9	The Influence of Radiation and Multivalent Cation Additions on Phase Separation and Crystallization of Glass
55188-DC	B-93	Chemical Decomposition of High-Level Nuclear Waste Storage/Disposal Glasses Under Irradiation
55367-IL	B-123	Investigation of Microscopic Radiation Damage in Waste Forms Using ODNMR and AEM Techniques
55382-IL	B-129	Determination of Transmutation Effects in Crystalline Waste Forms
54691-MI	B-189	Radiation Effects on Materials in the Near-Field of Nuclear Waste Repository
54672-WA	B-365	Radiation Effects in Nuclear Waste Materials

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55380-IL	B-127	In-Situ Spectro-Electrochemical Studies of Radionuclide Contaminated Surface Films on Metals and the Mechanism of their Formation and Dissolution
55387-NM	B-237	Photooxidation of Organic Wastes Using Semiconductor Nanoclusters
60401-SC	B-293	Mechanism of Pitting Corrosion Prevention by Nitrite in Carbon Steel Exposed to Dilute Salt Solutions
59925-WV	B-403	Modeling of Diffusion of Plutonium in Other Metals and of Gaseous Species in Plutonium-Based Systems

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54773-NM	B-215	Microstructural Properties of High Level Waste Concentrates and Gels with Raman And Infrared Spectroscopies
60363-NM	B-241	Optimization of Thermochemical, Kinetic, and Electrochemical Factors Governing Partitioning of Radionuclides during Melt Decontamination of Radioactively Contaminated Stainless Steel

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55105-MI	B-183	Complete Detoxification of Short Chain Chlorinated Aliphatics: Isolation of Halorespiring Organisms and Biochemical Studies of the Dehalogenating Enzyme Systems

Microbial Genetics and Instrumentation

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55152-MD	B-171	Molecular Profiling of Microbial Communities from Contaminated Sources: Use of Subtractive Cloning Methods and rDNA Spacer Sequences
55031-WA	B-373	Genetic Analysis of Stress Responses in Soil Bacteria for Enhanced Bioremediation of Mixed Contaminants
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54681-CA	B-67	Dynamics of Coupled Contaminant and Microbial Transport in Heterogeneous Porous Media
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Plant Genetics

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54837-GA	B-109	Phytoremediation of Ionic and Methyl Mercury Pollution

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54898-AZ	B-5	Molecular Dissection of the Cellular Mechanisms Involved in Nickel Hyperaccumulation in Plants
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60271-NH	B-199	Characterization of a New Family of Metal Transport Proteins

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54889-WA	B-389	Using Trees to Remediate Groundwaters Contaminated with Chlorinated Hydrocarbons

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54661-DE	B-91	Electrochemical Processes for In-Situ Treatment of Contaminated Soils
60313-IL	B-135	Radiation Effects on Transport and Bubble Formation in Silicate Glasses
59993-NM	B-223	Dynamic Effects of Tank Waste Aging on Radionuclide-Complexant Interactions
59982-NY	B-259	Reactivity of Peroxynitrite: Implications for Hanford Waste Management and Remediation
54122-PA	B-281	A Broad Spectrum Catalytic System for Removal of Toxic Organics from Water By Deep Oxidation
55103-TN	B-311	Utilization of Kinetic Isotope Effects for the Concentration of Tritium
54996-WA	B-371	Ionizing Radiation Induced Catalysis on Metal Oxide Particles
60392-WA	B-383	Radiolytic and Thermal Process Relevant to Dry Storage of Spent Nuclear Fuels
60050-WA	B-395	Chemical Speciation of Inorganic Compounds under Hydrothermal Conditions

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55012-CO	B-89	Extraction and Recovery of Mercury and Lead from Aqueous Waste Streams Using Redox-active Layered Metal Chalcogenides
54716-DC	B-97	Polyoxometalates for Radioactive Waste Treatment
60283-IL	B-133	Waste Volume Reduction Using Surface Characterization and Decontamination by Laser Ablation
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54791-KS	B-153	Managing Tight-binding Receptors for New Separations Technologies
54571-MA	B-181	Removal of Heavy Metals and Organic Contaminants from Aqueous Streams by Novel Filtration Methods
55223-MO	B-197	De Novo Design of Ligands for Metal Separation
54770-NM	B-213	New Anion-Exchange Resins for Improved Separations of Nuclear Materials
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55087-TN	B-309	Design and Synthesis of the Next Generation of Crown Ethers for Waste Separations: An Inter-Laboratory Comprehensive Proposal
60096-TN	B-339	Rational Synthesis of Imprinted Organofunctional Sol-Gel Materials for Toxic Metal Separation
54735-TX	B-343	Development of Inorganic Ion Exchangers for Nuclear Waste Remediation
60123-WA	B-397	Potential-Modulated Intercalation of Alkali Cations into Metal Hexacyanoferrate Coated Electrodes

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60017-PA	B-285	Removal of Technetium, Carbon Tetrachloride, and Metals from DOE Properties

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55152-MD	B-171	Molecular Profiling of Microbial Communities from Contaminated Sources: Use of Subtractive Cloning Methods and rDNA Spacer Sequences
55164-AL	B-3	Advanced Experimental Analysis of Controls on Microbial Fe(III) Oxide Reduction
55171-PA	B-283	Development of Advanced In-Situ Techniques for Chemistry Monitoring and Corrosion Mitigation in SCWO Environments
55179-NY	B-267	Acoustic Probe for Solid-Gas-Liquid Suspensions
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55188-DC	B-93	Chemical Decomposition of High-Level Nuclear Waste Storage/Disposal Glasses Under Irradiation
55196-OR	B-277	In Situ, Field Scale Evaluation of Surfactant Enhanced DNAPL Recovery Using a Single-Well, Push-Pull Test
55205-SC	B-299	A Fundamental Study of Laser-Induced Breakdown Spectroscopy Using Fiber Optics for Remote Measurements of Trace Metals
55211-IL	B-141	Cavitational Hydrothermal Oxidation: A New Remediation Process
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55300-MA	B-179	3-D Spectral IP Imaging: Non-Invasive Characterization of Contaminant Plumes
55318-CA	B-23	Improved Analytical Characterization of Solid Waste-Forms by Fundamental Development of Laser Ablation Technology
55328-TN	B-337	Novel Analytical Techniques Based on an Enhanced Electron Attachment Process
55332-NM	B-235	A Hybrid Hydrologic-Geophysical Inverse Technique for the Assessment and Monitoring of Leachates in the Vadose Zone
55343-CA	B-25	Enzyme Engineering for Biodegradation of Chlorinated Organic Pollutants
55351-CA	B-27	Evaluation of Isotopic Diagnostics for Subsurface Characterization and Monitoring: Field Experiments at the TAN and RWMC (SDA) Sites, INEL
55356-CA	B-29	Environmentally-induced Malignancies: An In Vivo Model to Evaluate the Health Impact of Chemicals in Mixed Waste
55359-CA	B-31	Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone

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Index of Research Awards by ID Number Continued

Among the environmental pollution scenarios that are particularly troublesome to the standard separation and purification methodologies are (1) those involving extremely dilute streams of radioactive or RCRA elements and (2) those in which such substances are absorbed in soils. In both cases, tight-binding, adequately selective, receptors offer the possibility of effective new technologies. For case (1) large binding constants are essential because of the effect of the high dilution; i.e., the moderate affinities of the receptors used in traditional solvent extraction or ion exchange methodologies may not assure binding. In the case of pollutants in soils, chemical binding to soil components or the presence of mineral forms can offer strong competition to any but the strongest of competing receptors.

The methodology for using tight-binding ligands in contaminated soil remediation draws on an analogy with the ligands called siderophores that are secreted by certain bacteria in order to salvage iron from the soil. A very powerful ligand is excreted across the cell membrane into the soil. The ligand diffuses with the aid of moisture and dissolves iron from its mineral forms. The complex formed by the iron is then recognized by the membrane and drawn back into the cell. In our scenario, the selective tight-binding ligand of choice is sprayed into the irrigated soil in the presence of a templated macroporous polymer that has been imprinted for the complex of interest. The ligand binds the metal ion, and the complex diffuses to the polymer and is bound. The polymer beads are removed from the soil, either by flotation, magnetically, or some other physical means, and the metal ion is released from the polymer-bound ligand and converted to a concentrated waste form.

The full list of Environmental Management projects that could potentially be addressed by projects such as this one, which deals with Mixed Waste problems, are listed in the Index of High Cost Environmental Management Projects by Problem Area, in the back of this appendix, under the heading "Mixed Waste".

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Report to Congress on the U.S. Department of Energy's Environmental Management Science Program

Research Funded and Its Linkages to Environmental Cleanup Problems

Environmental Management Science Program Research Award Abstracts

Volume II of III
Appendix B

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